Support Vector Machines

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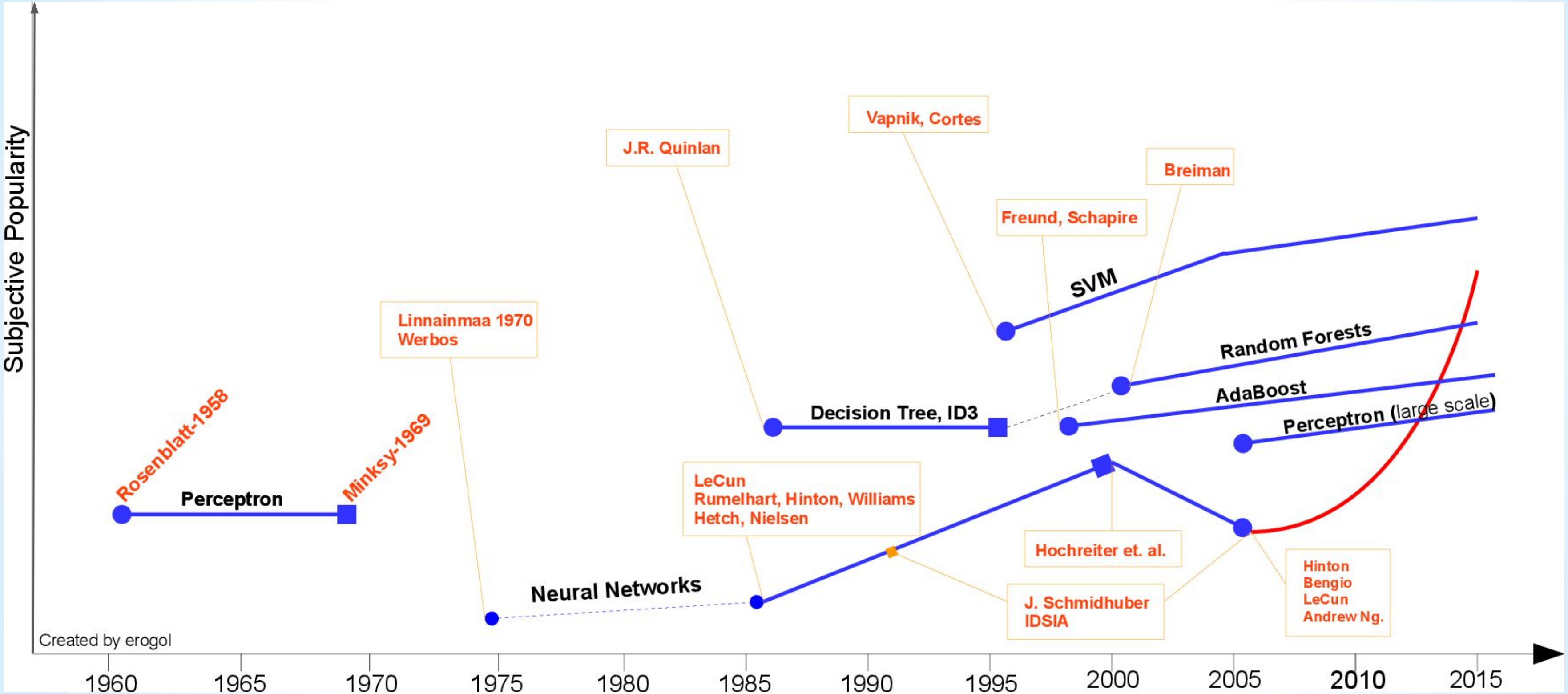
Models History

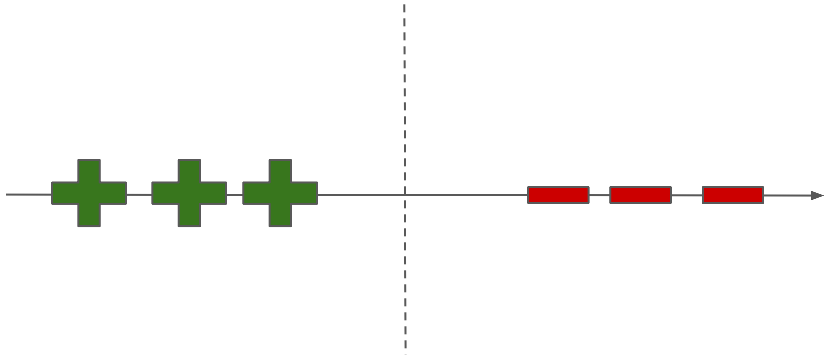


Motivation

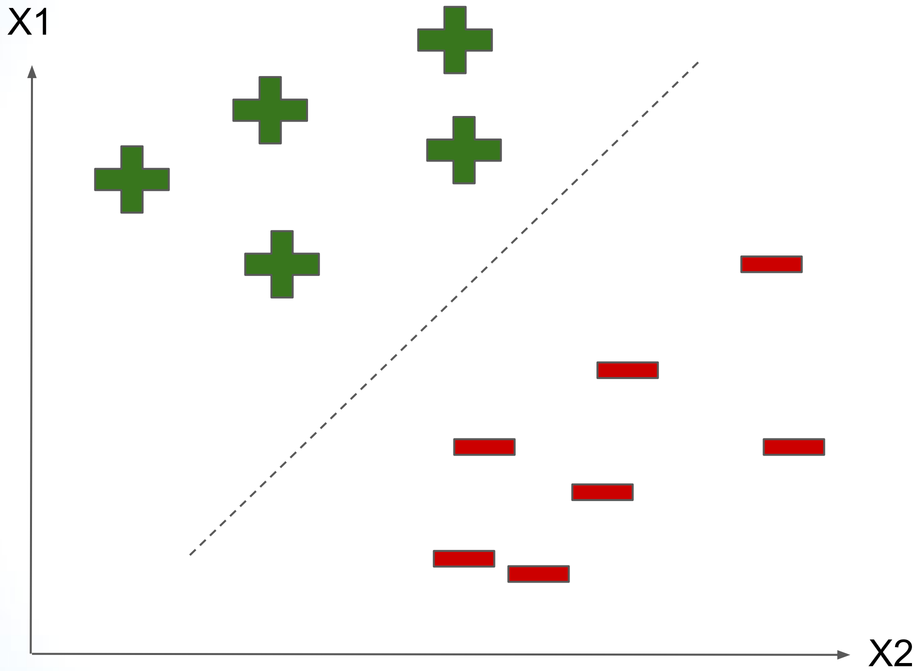
Good for difficult problems with limited data (<10K data points)

- Face Detection
- Text Classification
- Protein Fold and Remote Homology Detection
- Handwriting Recognition

Linear Classification - 1 dim



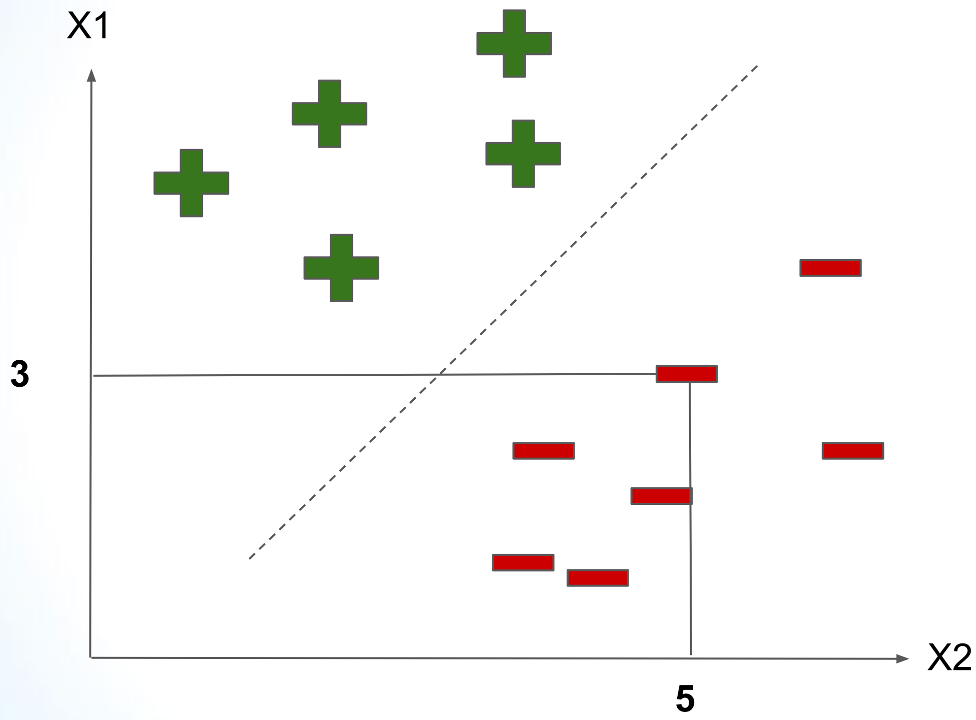
Linear Classification - 2 dim



w1*x1 = w2*x2 + b

2*x1 = 4*x2 - 3
2*x1 - 4*x2 + 3 = 0

Linear Classification - 2 dim

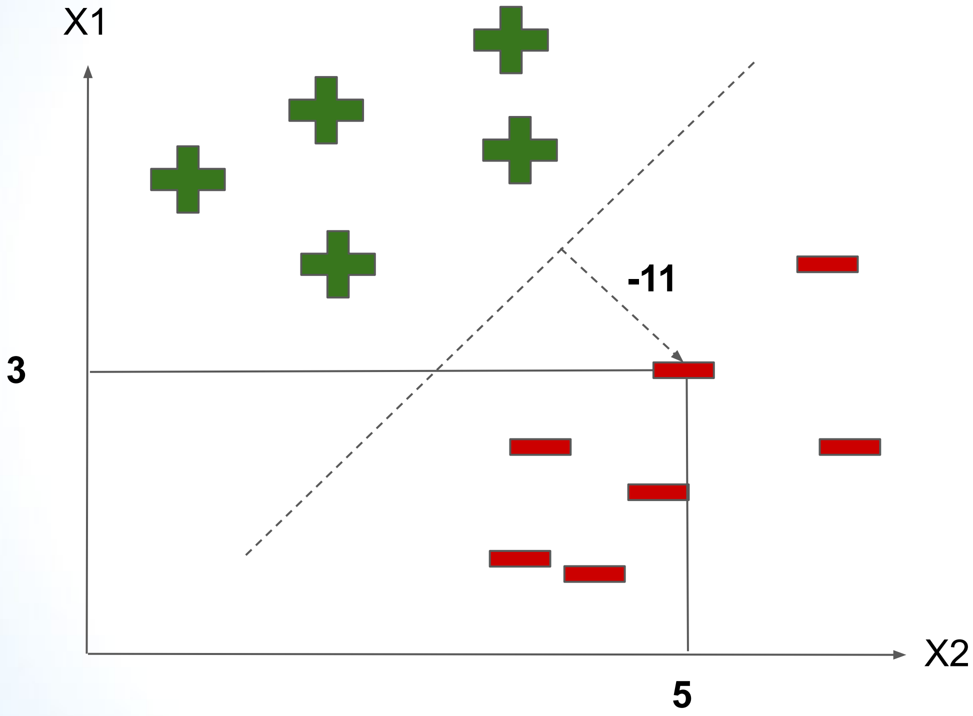


w1*x1 = w2*x2 + b

2*x1 = 4*x2 - 3
2*x1 - 4*x2 + 3 = 0

2*3 - 4*5 + 3 =

Linear Classification - 2 dim



w1*x1 = w2*x2 + b

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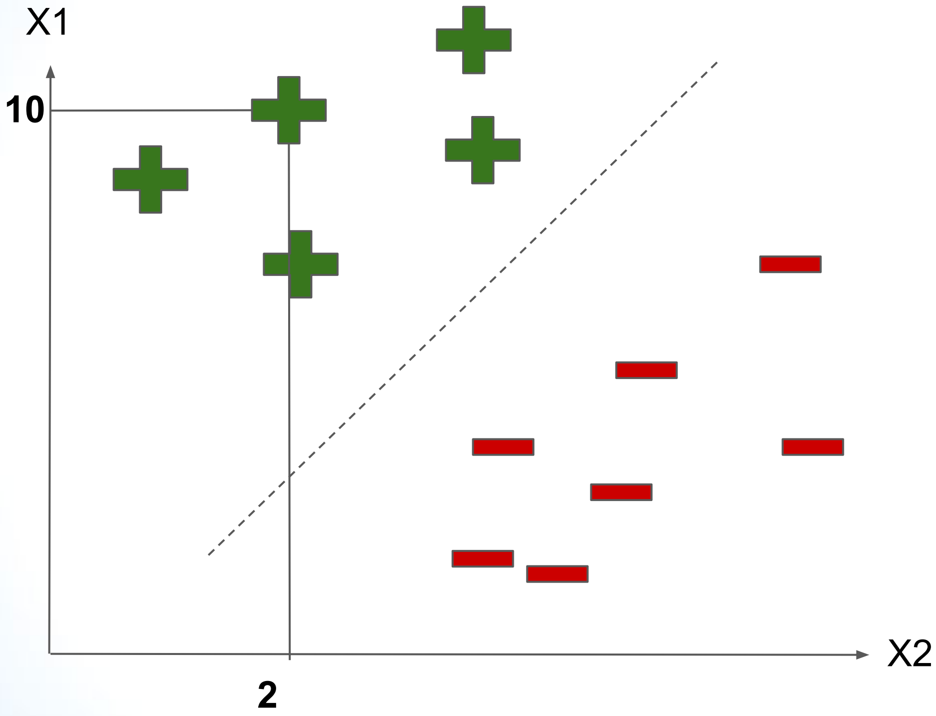
2*x1 - 4*x2 + 3 = 0

2*3 - 4*5 + 3 = 6 - 20 + 3 = -11

Linear Classification - 2 dim



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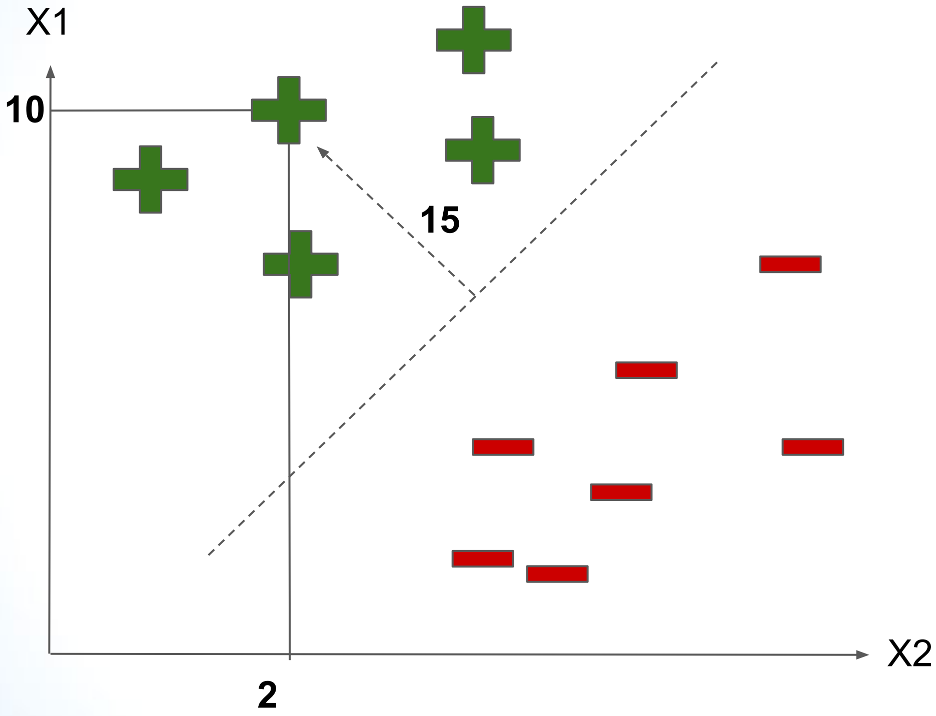
$2*10 - 4*2 + 3 = 20 - 8 + 3 = 15$

Linear Classification - 2 dim



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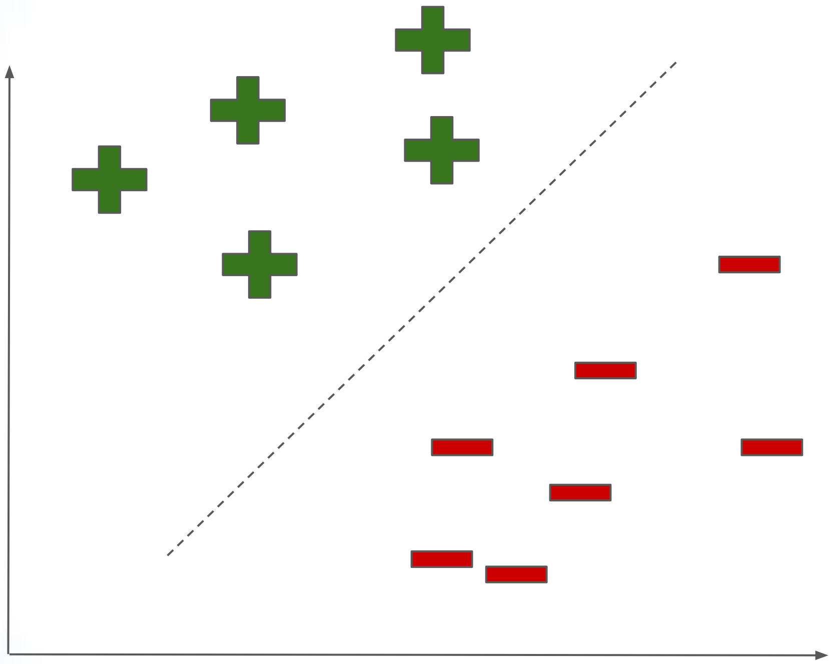
Linear Classification - 2 dim

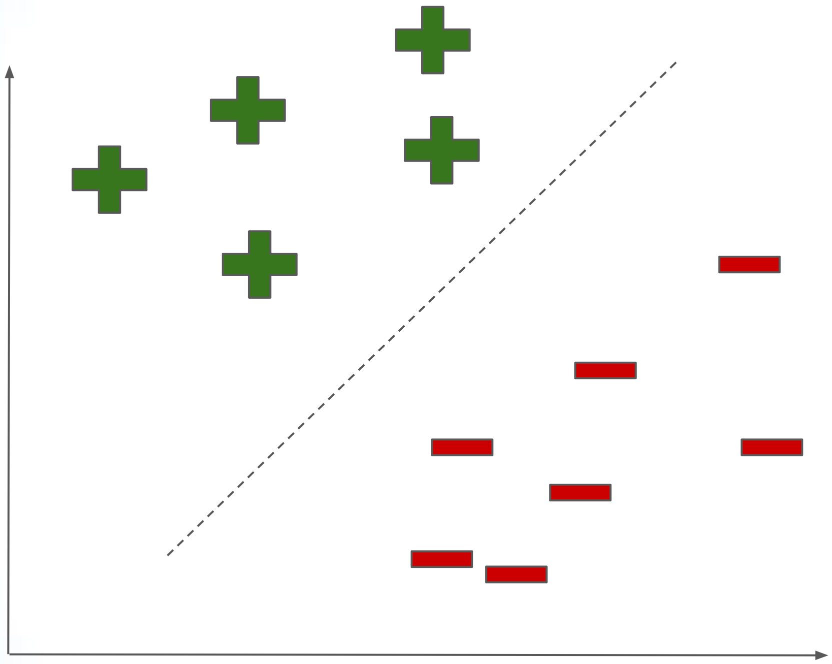


w1*x1 = w2*x2 + b

f(X,W) = w1*x1 + w2*x2 =

For simplicity We are going to eliminate the bias term Which can be added as a vectors of ones

Linear Classification - 2 dim

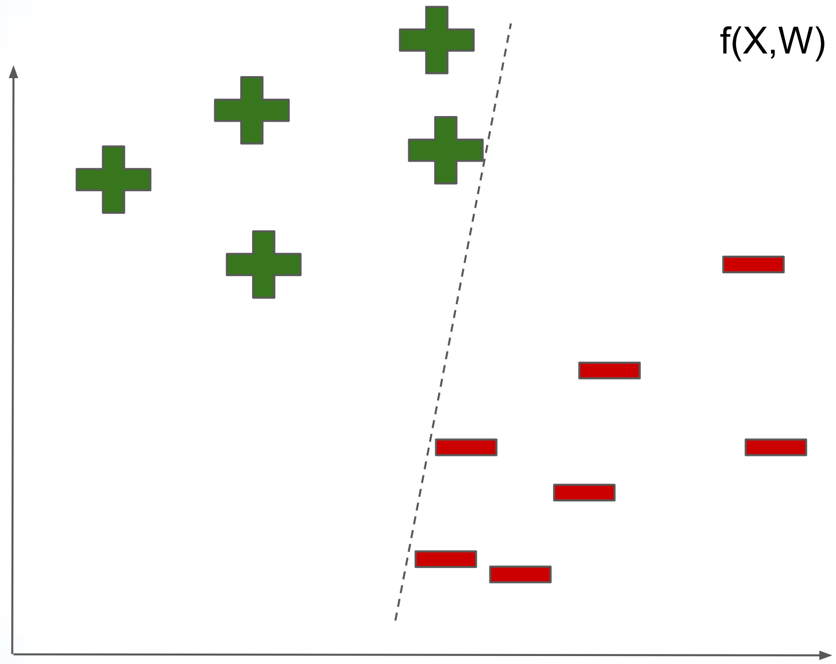


w1*x1 = w2*x2 + b

f(X,W) = w1*x1 + w2*x2 =
= ΣWX = W^{t}X = 0
=> sign(WX)

For simplicity We write
W^{t}X as WX

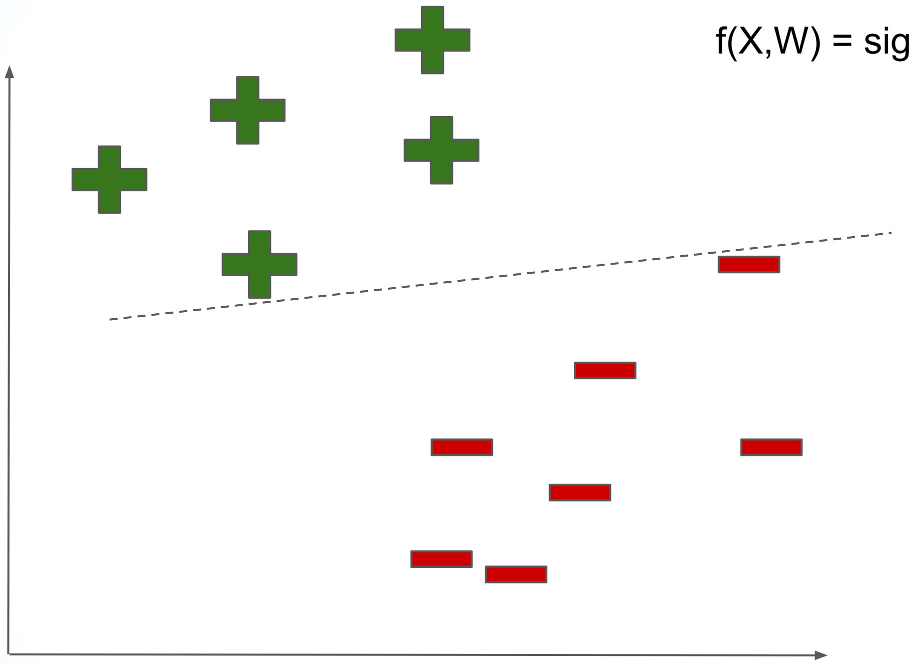
Linear Classification



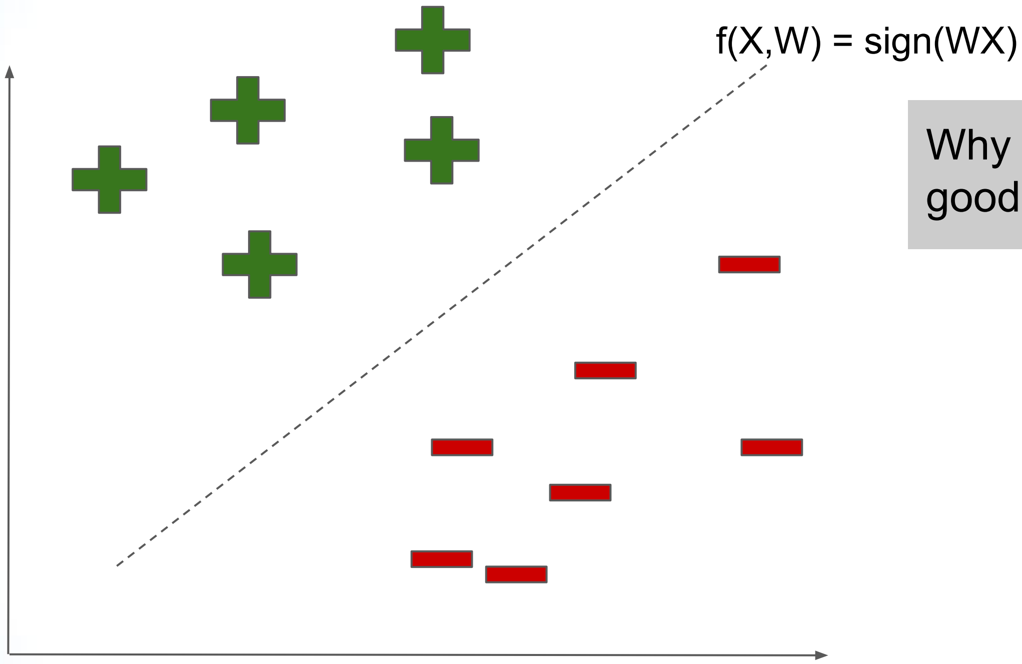
f(X,W) = sign(WX)

Linear Classification

$f(X,W) = \text{sign}(WX)$

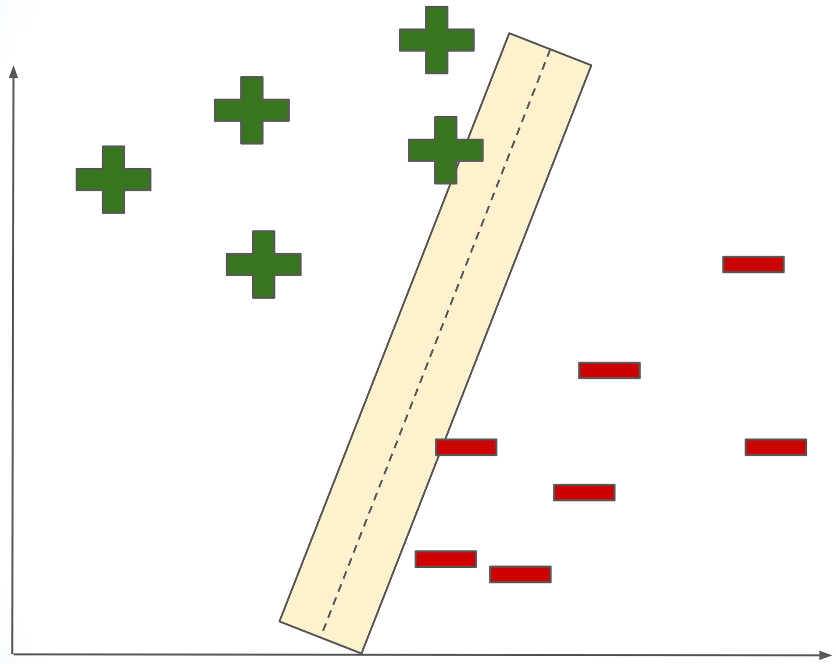


Linear Classification



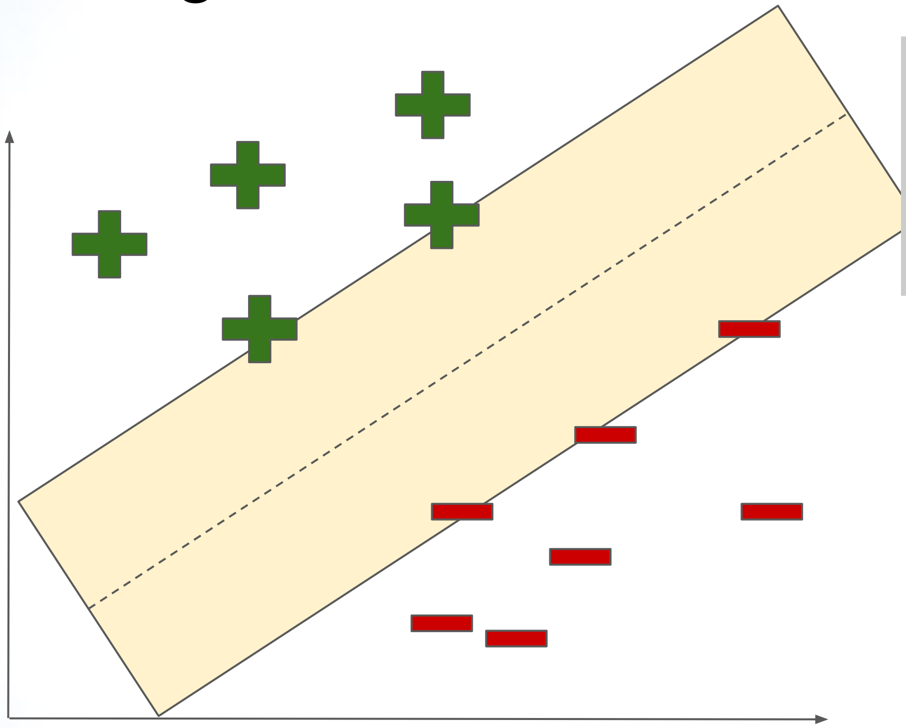
Why is this seems as a good separator?

Classifier Margin



A margin in linear classifiers is the boundary width the touches the datapoint

Maximum margin



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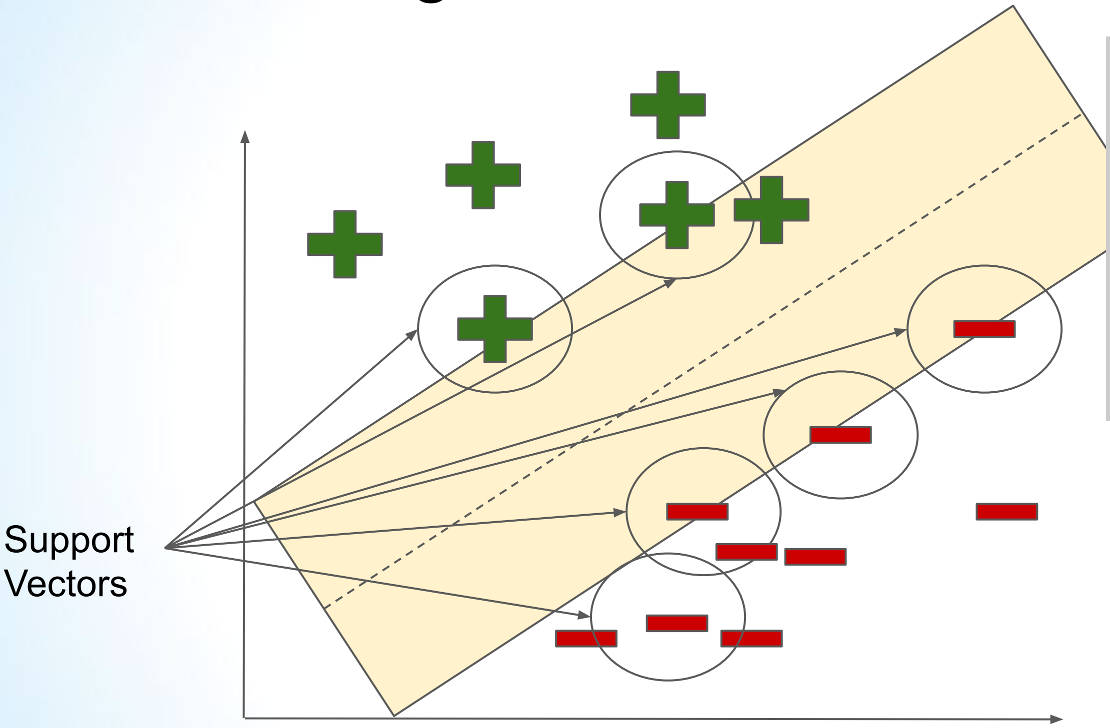
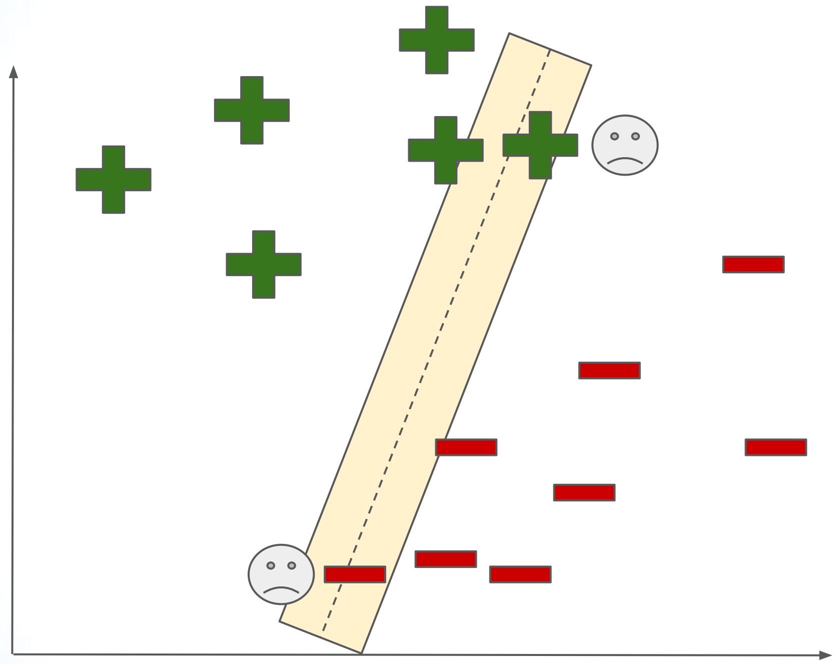
Maximum Margin



A maximum margin in linear classifiers is the Max boundary width the touches the datapoint

The points on the margins are called Support Vectors

Classifier Margin



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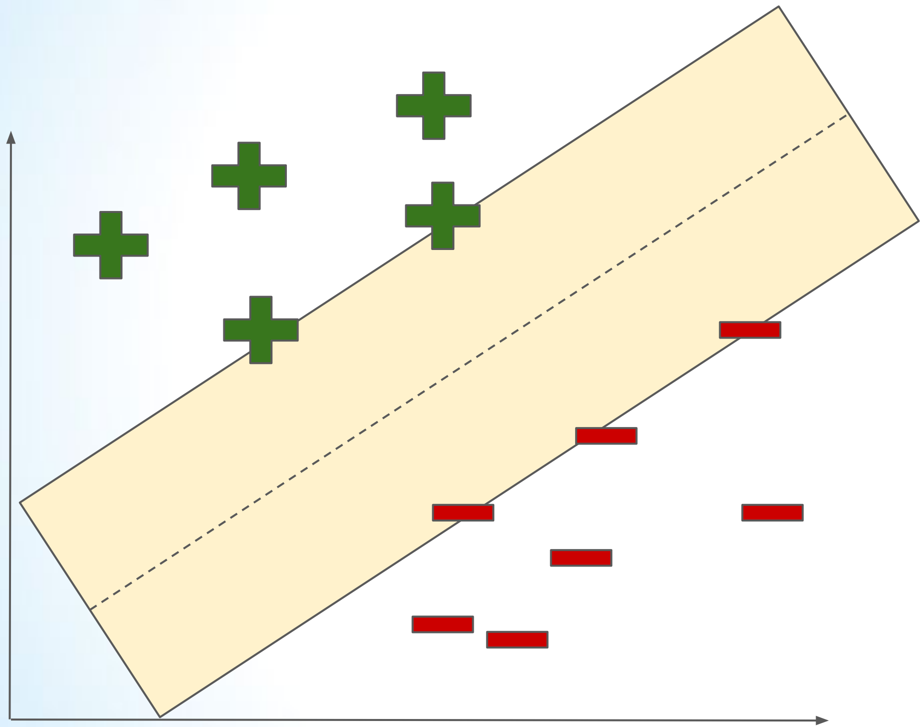
Allows a more flexibility around the decision boundary

Classifier Margin



A maximum margin in linear classifiers is the Max boundary width the touches the datapoint

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Allows a more flexibility around the decision boundary

VC dimension **can show that the maximum margin is a good approach to linearly separable problems.**

VC Dimension - Vapnik-Chervonenkis (60-90)

Explain learning from a statistical view

VC-dim measure the **capacity** of a learner

Complexity

Expressive power

Richness

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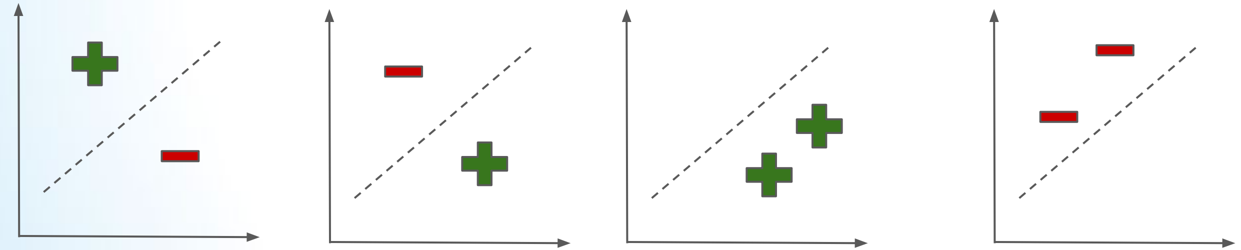
VC Dimension - Vapnik-Chervonenkis (60-90)

VC-dim is the maximum number of points the learner can **Shatter**

A learner can **Shatter** points if all y’s can achieve Zero error on the train set

Perceptron / logistic regression for 2 points:



1. Lets try 3 points   And 4..

2. What is the VC-dim of the learner? **dim + 1**   3. What happened with 3 points same line..

VC Dimension - Vapnik-Chervonenkis (60-90)

VC-dim can predict the probabilistic upper bound of the test error (!)

N: The training-set size

$$\Pr\left(\text{test error} \leqslant \text{training error} + \sqrt{\frac{1}{N}\left[D\left(\log\left(\frac{2N}{D}\right)+1\right)-\log\left(\frac{\eta}{4}\right)\right]}\right) = 1-\eta,$$

Valid When N >> D

$$0 < \eta \leqslant 1$$

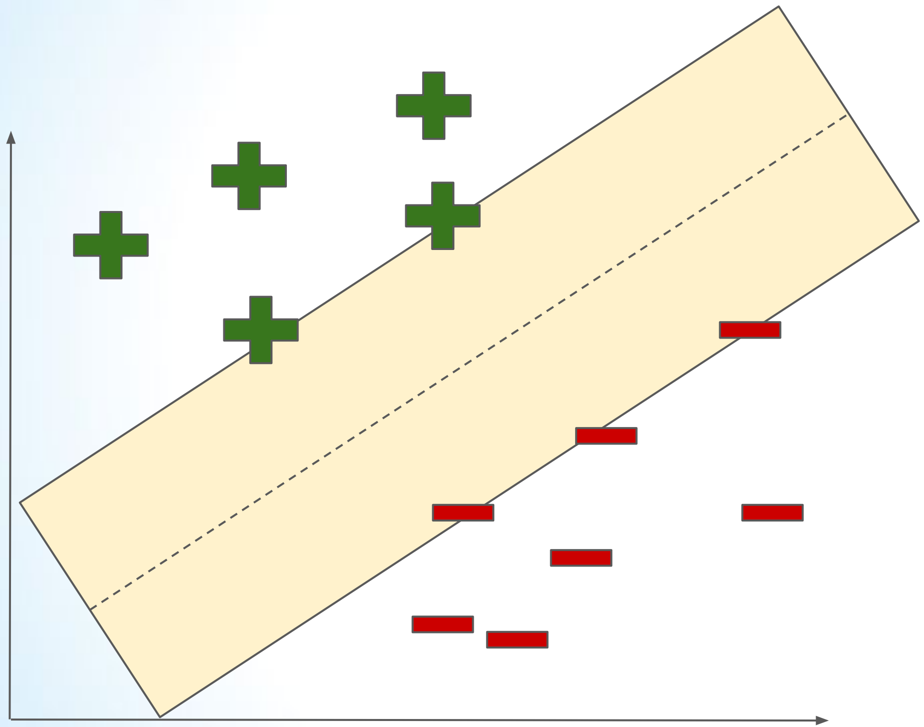
D: The VC-dim of a learner

$$D_{svm} = 1 + \frac{1}{margin^2}$$

In the linear separable case

Higher margin, lower D, lower test error

Classifier Margin



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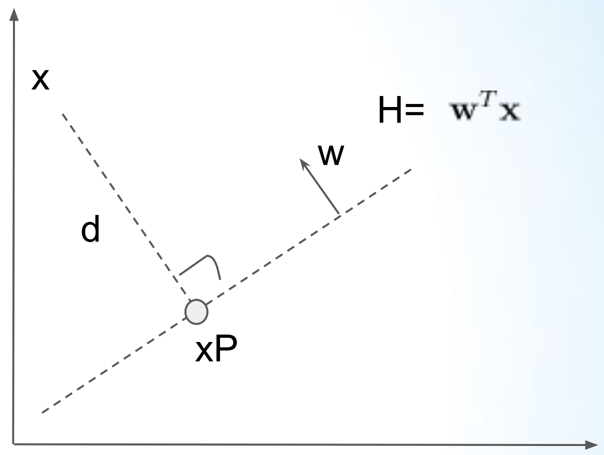
Hard SVM - the separable case

What is the distance between point X and the hyperplane?

- x is a point
- d vector from H to x with minimum length
- xP is the projection of x on H



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Defining the Margin

$$\mathbf{w}^T\mathbf{x}^P = 0 \qquad \mathbf{x}^P = \mathbf{x} - \mathbf{d} \qquad \mathbf{d} = \alpha\mathbf{w} \quad \alpha \in \mathbb{R}$$

XP is a point on H

d is parallel to w

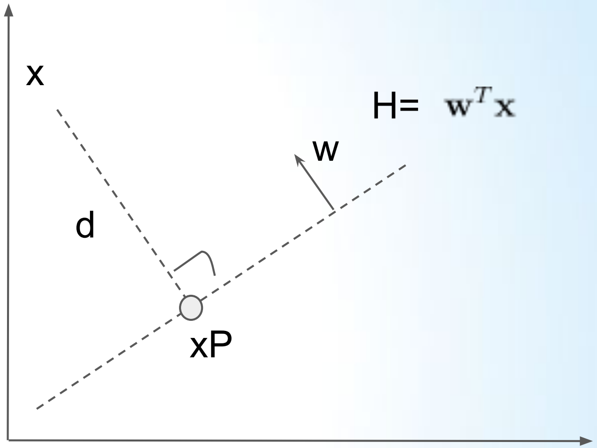
$$\mathbf{w}^T\mathbf{x}^P = \mathbf{w}^T(\mathbf{x} - \mathbf{d}) = \mathbf{w}^T(\mathbf{x} - \alpha\mathbf{w}) = 0$$

$$\alpha = \frac{\mathbf{w}^T\mathbf{x}}{\mathbf{w}^T\mathbf{w}}$$

The length of d: $\|\mathbf{d}\|_2 = \sqrt{\mathbf{d}^T\mathbf{d}} = \sqrt{\alpha^2\mathbf{w}^T\mathbf{w}} = \frac{|\mathbf{w}^T\mathbf{x}|}{\sqrt{\mathbf{w}^T\mathbf{w}}} = \frac{|\mathbf{w}^T\mathbf{x}|}{\|\mathbf{w}\|_2}$

Margin of H with respect to D: $\gamma(\mathbf{w}) = \min_{\mathbf{x}\in D} \frac{|\mathbf{w}^T\mathbf{x}|}{\|\mathbf{w}\|_2}$

By definition, the margin and hyperplane are scale invariant: $\gamma(\beta\mathbf{w}) = \gamma(\mathbf{w}), \forall\beta \neq 0$



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Defining the Maximum Margin

$$\underbrace{\max_{\mathbf{w}} \gamma(\mathbf{w}, b)}_{maximize\ margin} \text{ such that } \underbrace{\forall i\ y_i(\mathbf{w}^T x_i) \geq 0}_{separating\ hyperplane}$$

$$\underbrace{\max_{\mathbf{w}} \underbrace{\frac{1}{\|\mathbf{w}\|_2} \min_{\mathbf{x}_i \in D} \left|\mathbf{w}^T \mathbf{x}_i\right|}_{\gamma(\mathbf{w})}}_{maximize\ margin} \quad s.t. \quad \underbrace{\forall i\ y_i(\mathbf{w}^T x_i) \geq 0}_{separating\ hyperplane}$$

Because the hyperplane is scale invariant, we can fix the scale of w anyway we want. Let's be clever about it, and choose it such that

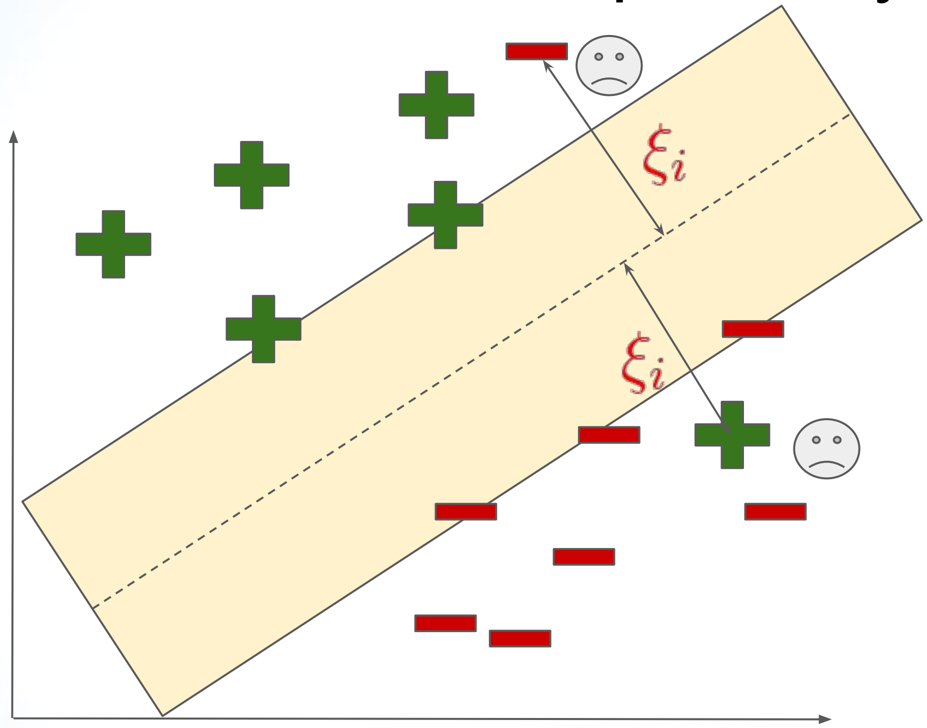
$$\min_{\mathbf{x} \in D} \left|\mathbf{w}^T \mathbf{x}\right| = 1.$$

$$\max_{\mathbf{w}} \frac{1}{\|\mathbf{w}\|_2} \cdot 1 = \min_{\mathbf{w}} \|\mathbf{w}\|_2 = \min_{\mathbf{w}} \mathbf{w}^\top \mathbf{w} \qquad \text{s.t.} \quad \forall i\ y_i(\mathbf{w}^T \mathbf{x}_i) \geq 1$$

$$\boxed{min_w \|w\|^2 \ \ s.t \ \ \forall i, y_i w x_i \geq 1}$$

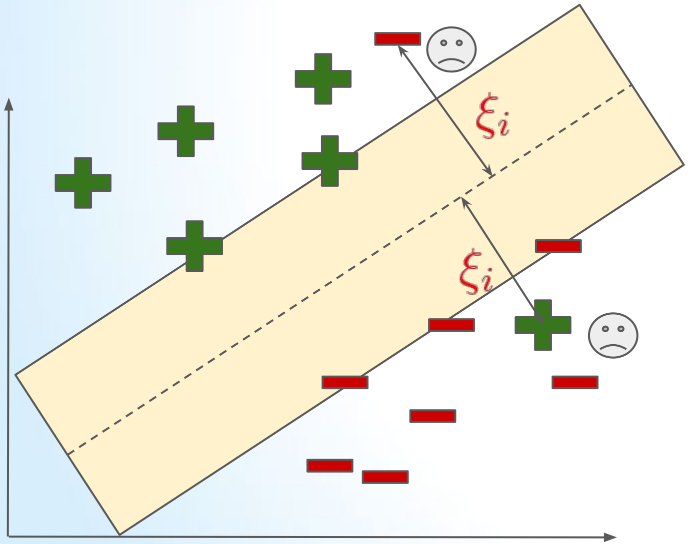
*Assumes full separability

What if there is no linear separability?



Soft SVM - Supporting error data points

$$argmin_{w,\xi}\left(\lambda\left\|w\right\|^2+C\frac{1}{m}\sum_{i=1}^{m}\xi_i\right)$$



$$s.t\ \forall y_i(wx_i) >= 1-\xi_i$$

Soft SVM - Supporting error data points

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$$argmin_{w,\xi}\left(\lambda\left\|w\right\|^2 + \underbrace{hinge(wx,y)}_{max\left\{0,1-ywx\right\}}\right)$$

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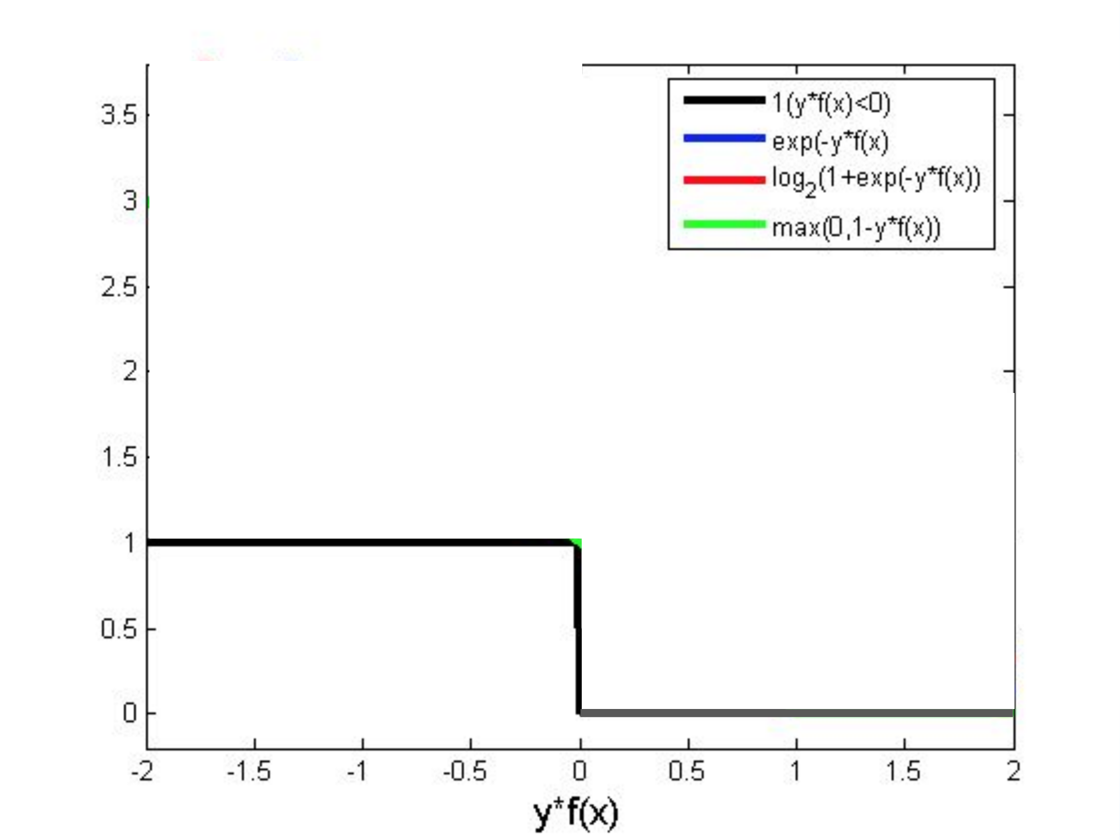
regularization objective

But came from problem definition

Draw me a function



Soft SVM - Supporting error data points

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$$argmin_{w,\xi}\left(\lambda\left\|w\right\|^2 + \underbrace{hinge(wx,y)}_{max\{0,1-ywx\}}\right)$$

regularization objective

But came from problem definition

How we can solve it?

Gradient descent

Quadratic Programing

```
SGD for solving Soft-SVM
```

goal: Solve $\operatorname{argmin}_{\mathbf{w}} \left(\frac{\lambda}{2}\|\mathbf{w}\|^2 + \frac{1}{m}\sum_{i=1}^{m} \max\{0, 1 - y\langle \mathbf{w}, \mathbf{x}_i \rangle\} \right)$

parameter: T

initialize: $\boldsymbol{\theta}^{(1)} = \mathbf{0}$

for $t = 1, \ldots, T$

  Let $\mathbf{w}^{(t)} = \frac{1}{\lambda t}\boldsymbol{\theta}^{(t)}$

  Choose i uniformly at random from $[m]$

  If $(y_i\langle \mathbf{w}^{(t)}, \mathbf{x}_i \rangle < 1)$

    Set $\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + y_i \mathbf{x}_i$

  Else

    Set $\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)}$

output: $\bar{\mathbf{w}} = \frac{1}{T}\sum_{t=1}^{T} \mathbf{w}^{(t)}$

https://leon.bottou.org/publications/pdf/lin-2006.pdf

Homework

1. **Implementing SVM called Pegasos (2011) - 55 (+ 10 bonus)**
   1. Implement Class - 35
   2. Test - 10
   3. Analyze param - 5
   4. Analyze learning - 5
   5. Mini-batch bonus - 10*
2. **The effect of imbalance on SVM** - **15**
3. **Practical SVM in scikit-learn & hypertune - 10**
4. **Using different Kernels - 20**

Another Way to Solve SVM

And other tricks

From Primal to Dual

Primal

$$min\ \ f_0(x)$$

$$s.t\ \ f_i(x) \le 0 \quad \forall i = 1..m$$

Original SVM definition

From Primal to Dual

Primal

$$min\ \ f_0(x)$$

$$s.t\ \ f_i(x) \leq 0 \quad \forall i = 1..m$$

Original SVM definition

Dual

$$L_{\alpha \geq 0}(x, \alpha) = f_0(x) + \sum_{i=1} \alpha_i f_i(x)$$

$$g(\alpha) = min_x\ \ L(x, \alpha)$$

Dual definition that solvable with **linear solvers**

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From Primal to Dual

Primal

$$\min f_0(x)$$

$$s.t\ f_i(x) \leq 0 \quad \forall i = 1..m$$

Dual

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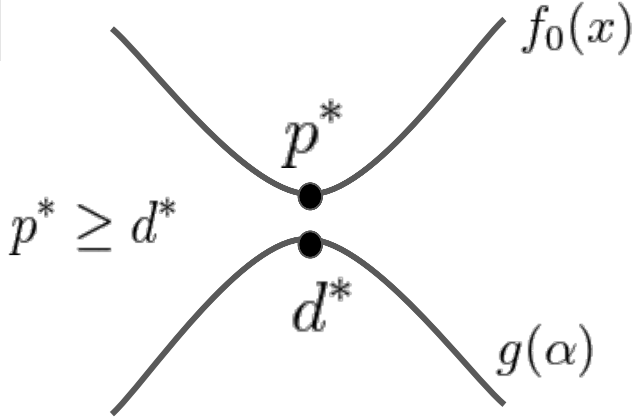

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$$g(x) = min_x \;\; L(x, \alpha)$$

SVM definition

$$min \;\; \|w\|^2$$

$$s.t \quad y_i w x_i \geq 1 \;\; \forall i = 1..m$$

From Primal to Dual

Primal

$$min\ f_0(x)$$

$$s.t\ f_i(x) \leq 0 \quad \forall i = 1..m$$

SVM definition

$$min\ \|w\|^2$$

$$s.t \quad y_i w x_i \geq 1 \ \ \forall i = 1..m$$

Modify

$$min\ \frac{1}{2}\|w\|^2$$

$$s.t \quad 1 - y_i w x_i \leq 0 \ \ \forall i = 1..m$$

Dual

$$\underset{\alpha \geq 0}{L(x,\alpha)} = f_0(x) + \sum_{i=1}^{m} \alpha f_i(x)$$

$$g(x) = min_x\ L(x,\alpha)$$

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From Primal to Dual

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$$min\ \ f_0(x)$$

$$s.t\ \ f_i(x) \leq 0 \quad \forall i = 1..m$$

SVM definition

$$min\ \ \|w\|^2$$

$$s.t \quad y_i w x_i \geq 1 \ \ \forall i = 1..m$$

Modify

$$min\ \frac{1}{2}\|w\|^2$$

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Dual

$$\underset{\alpha \geq 0}{L(x, \alpha)} = f_0(x) + \sum_{i=1}^{m} \alpha f_i(x)$$

$$g(x) = min_x\ \ L(x, \alpha)$$

$$\underset{\alpha \geq 0}{L(x, \alpha)} = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i (y_i w x_i - 1)$$

$$g(\alpha) = min_x\ \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i (y_i w x_i - 1)$$

From Dual to Primal

$$\underset{\alpha \geq 0}{L(x, \alpha)} = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i (y_i w x_i - 1)$$

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From Dual to Primal

$$\underset{\alpha\geq 0}{L(x,\alpha)} = \frac{1}{2}\left\|w\right\|^2 - \sum_{i=1}^{m}\alpha_i(y_i w x_i - 1)$$

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$$\frac{\partial L}{\partial w} = 0$$

From Dual to Primal

$$\underset{\alpha \geq 0}{L(x, \alpha)} = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i (y_i w x_i - 1)$$

$$g(\alpha) = min_x \ \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i (y_i w x_i - 1)$$

$$\frac{\partial L}{\partial w} = 0$$

$$w - \sum_{i=1}^{m} \alpha_i y_i x_i = 0$$

$$w* = \sum_{i=1}^{m} \alpha_i y_i x_i$$

$$\alpha_i \geq 0$$

Lagrange coefficients for each sample in the training set

Optimization Definition	$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l x_k x_l$$	All possible pairs in the training set
Constraints	$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$	

Optimization Definition	$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l x_k x_l$$
Constraints	$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$
Back to Primal	$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$

Optimization Definition	$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l x_k x_l$
Constraints	$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$
Back to Primal	$w = \sum_{k=1}^{R} \alpha_k y_k x_k$
Predict	$f(x, w) = sign(w, x)$

Optimization Definition

$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l x_k x_l$$

Constraints

$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$

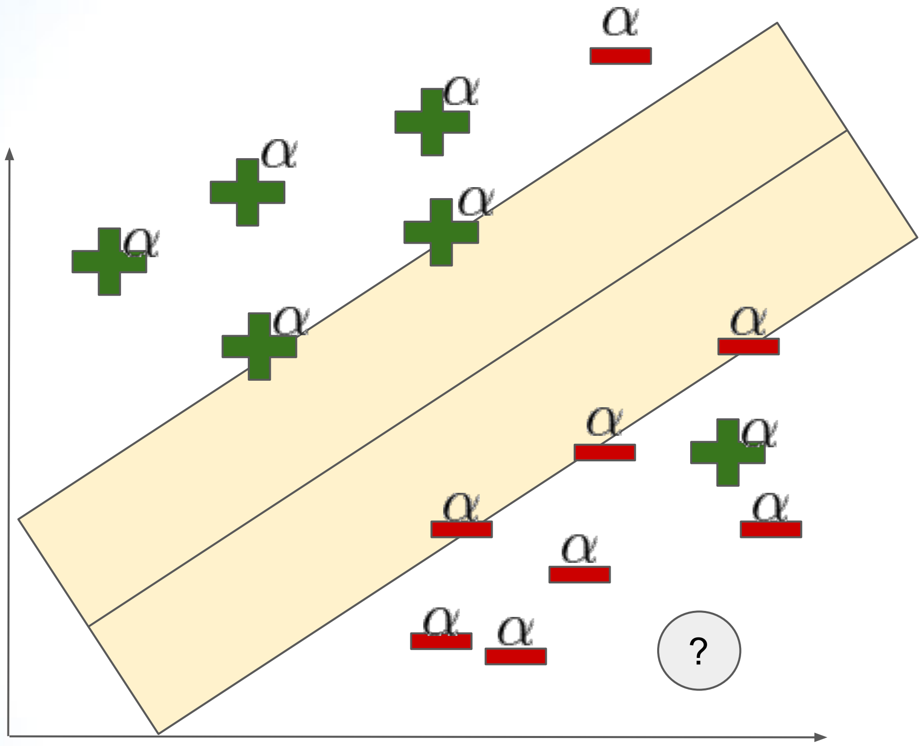
Back to Primal

$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$

Predict

$$f(x, w) = sign(w, x) \Longrightarrow f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

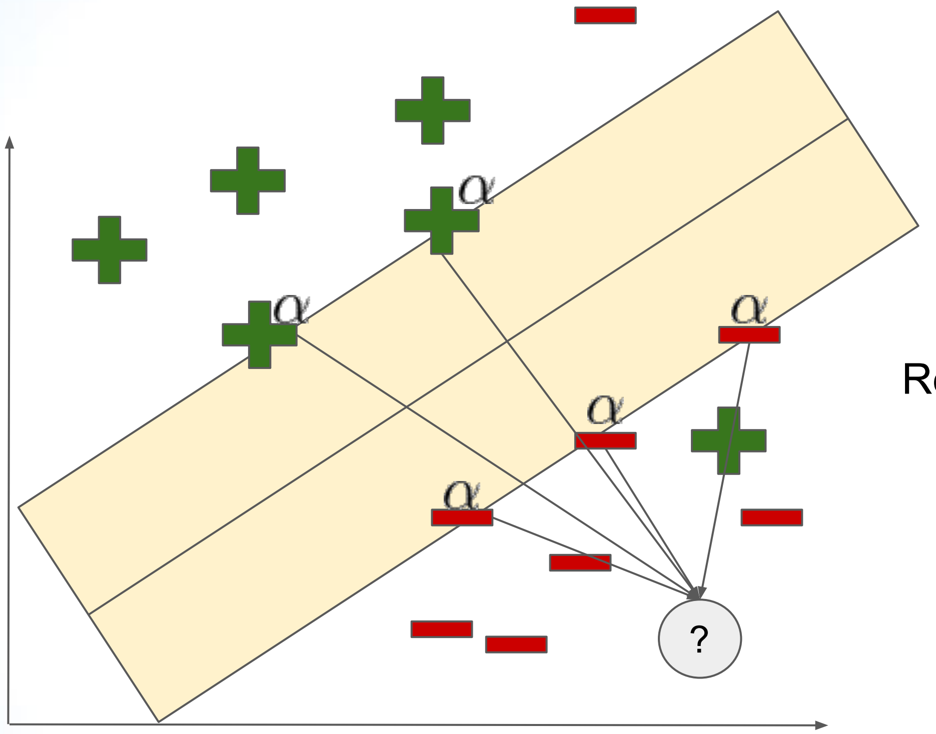
Applying



$$f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

- What is the alpha values on the margin?
- Outside the margin?

Applying

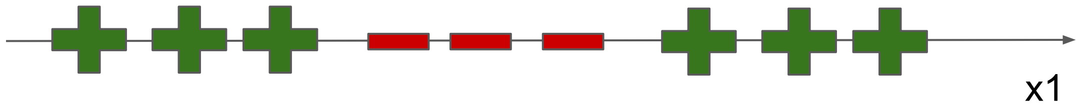


$$f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

Reminds you something?

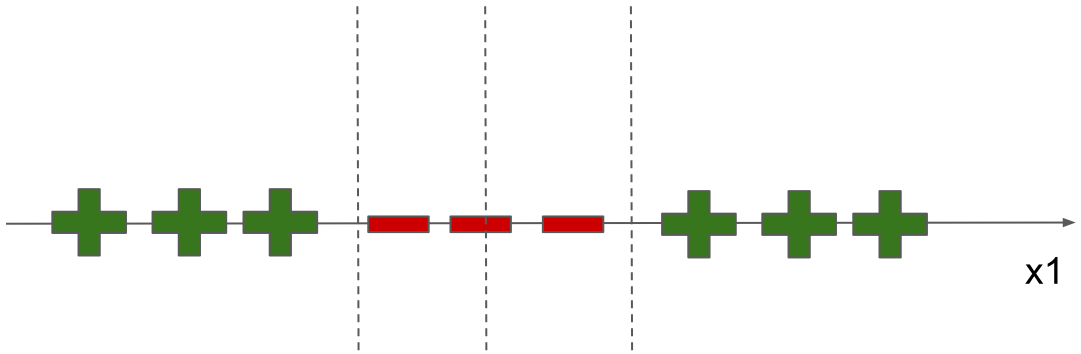
Dealing with non-linearity

How to separate with linear classifier?



Dealing with non-linearity

How to separate with linear classifier?



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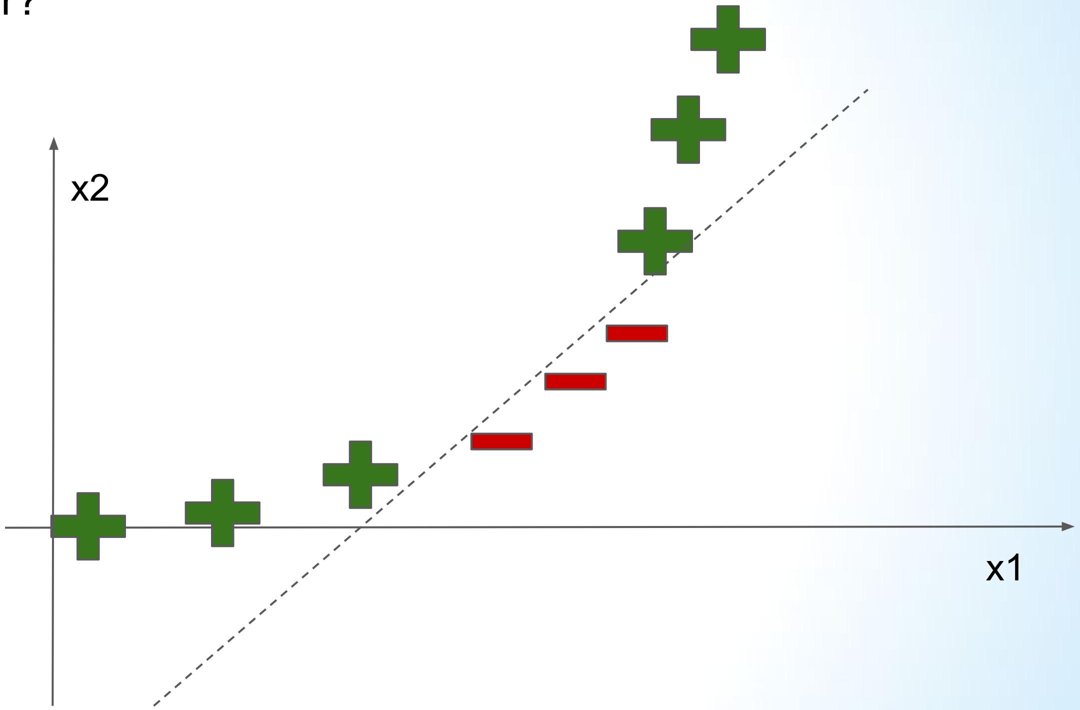
Dealing with non-linearity

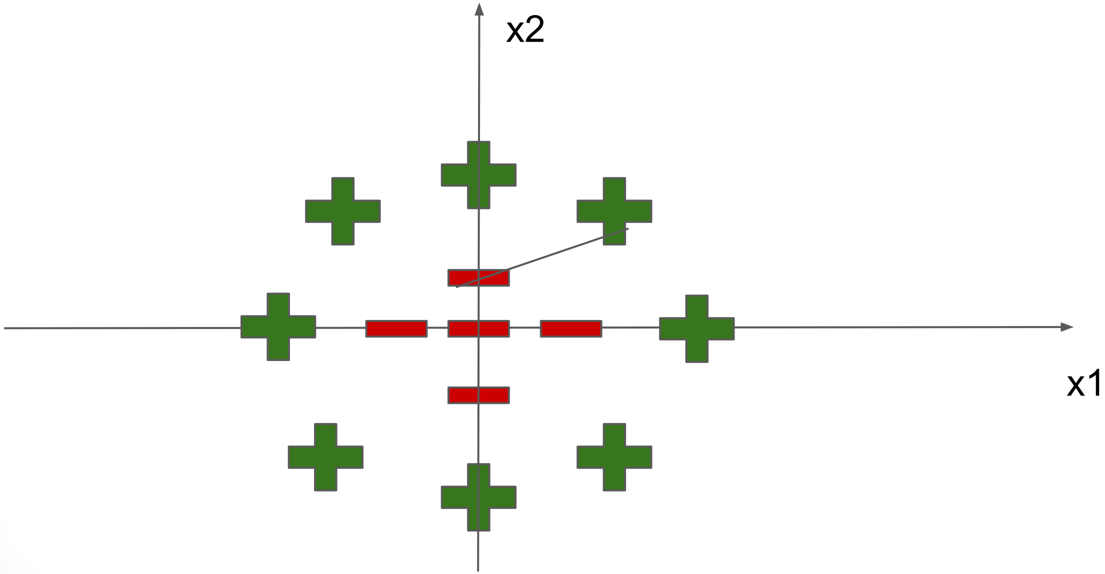
How to separate with linear classifier?

Use non-linear transformation

$$\phi(X) : \mathbb{R}^k \rightarrow \mathbb{R}^n | n > k$$

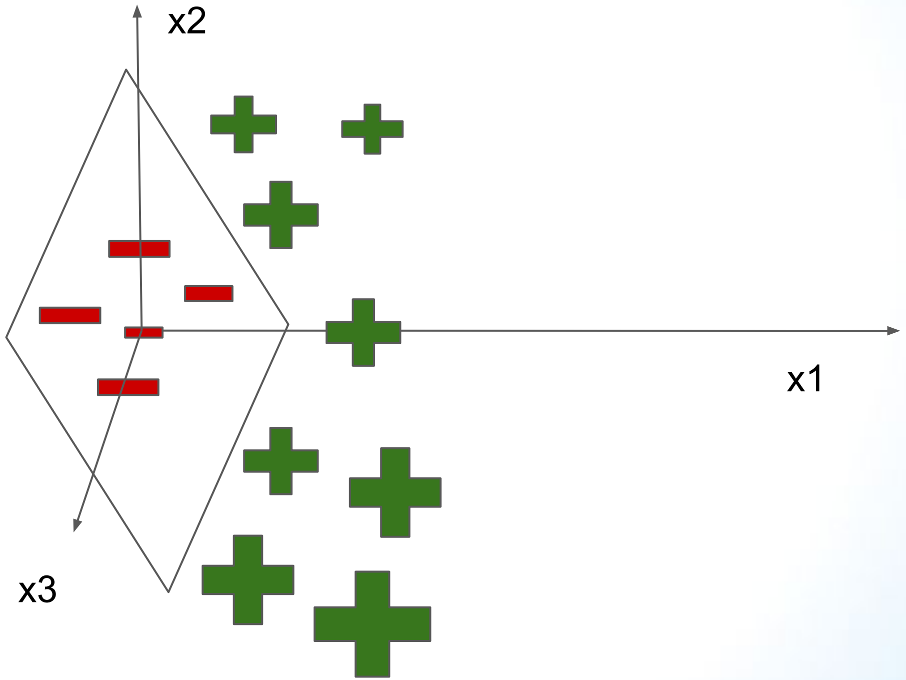


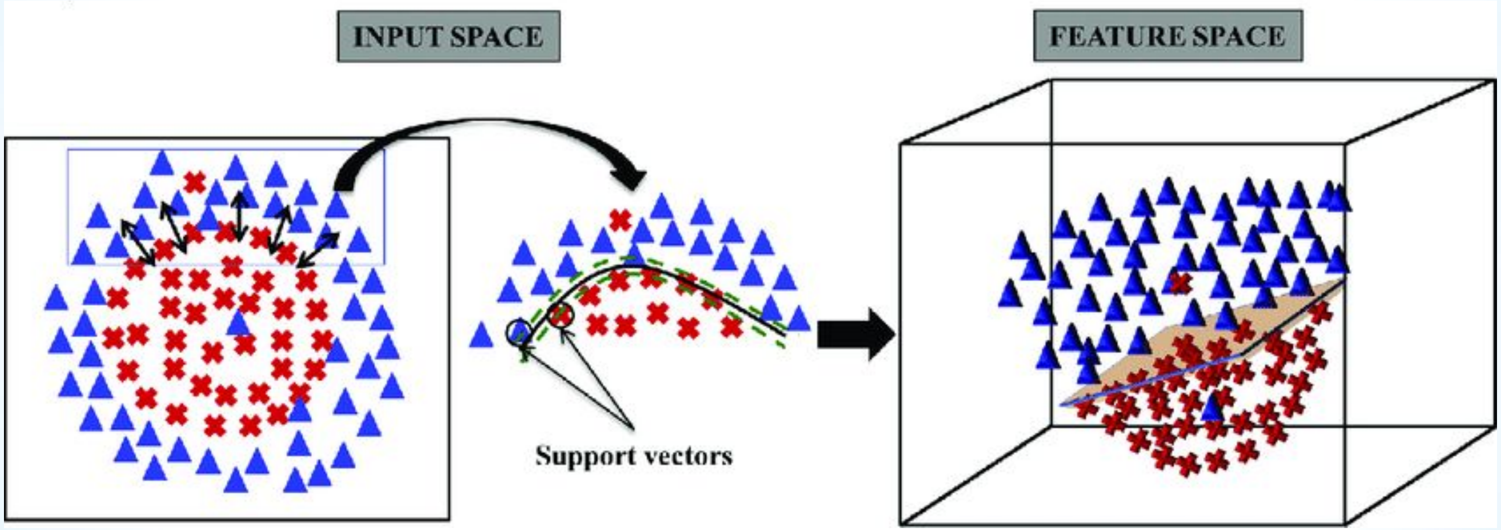
Dealing with non-linearity



Dealing with non-linearity

$$\phi(X) : \mathbb{R}^k \rightarrow \mathbb{R}^n | n > k$$




INPUT SPACE
FEATURE SPACE
Support vectors

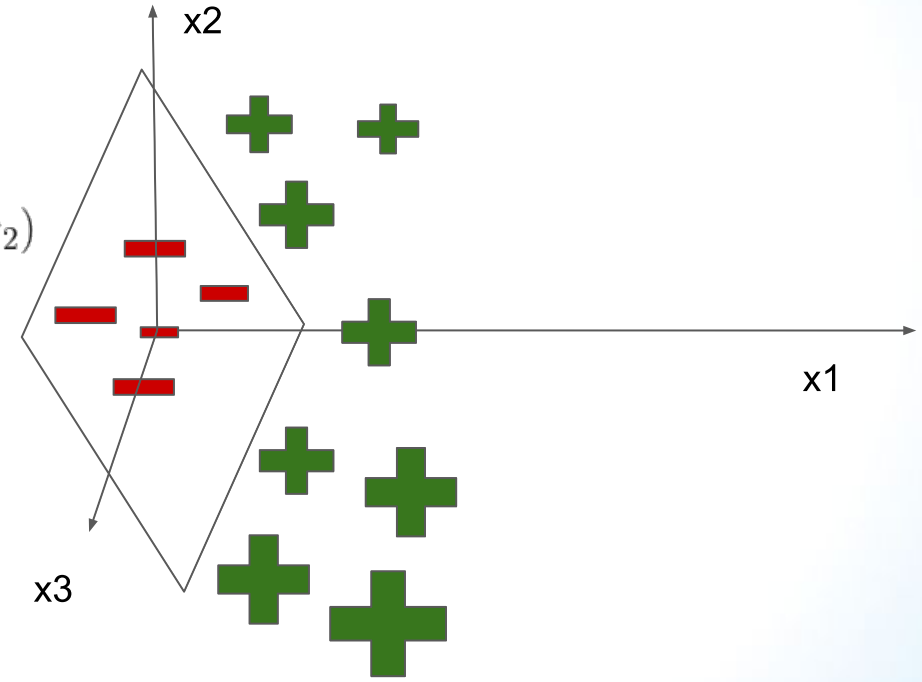
Dealing with non-linearity

How to separate with linear classifier?

$$\phi(X) : \mathbb{R}^k \rightarrow \mathbb{R}^n | n > k$$

$$(x_1, x_2) \mapsto \theta(X) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

A capital X = a datapoint



The Kernel Trick

To support this transformation We would need to compute all these features for each sample

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The Solution: the Kernel trick!
Use a dot product in feature space can be computed as kernel function

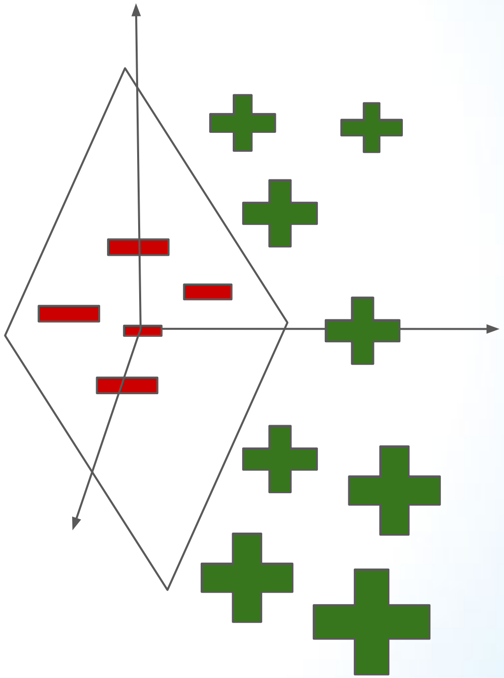
$$K(x_i, x_j) = \phi(x_i)\phi(x_j)$$

The Kernel Trick

$$(x_1, x_2) \mapsto \theta(X) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$K(X_i, X_j) = \phi(X_i)\phi(X_j) = (X_iX_j)^2$$

$$= (X_{i_1}^2, X_{i_2}^2, \sqrt{2}X_{i_1}X_{i_2})(X_{j_1}^2, X_{j_2}^2, \sqrt{2}X_{j_1}X_{j_2})^T =$$
$$(X_{i_1}X_{j_1} + X_{i_2}X_{j_2})^2 = (X_iX_j)^2$$



The Kernel Trick

We would need to compute all these features!

The Solution: the Kernel trick!
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Where do we have dot product in SVM?

Optimization Definition

$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l x_k x_l$$

Constraints

$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$

Back to Primal

$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$

Predict

$$f(x, w) = sign(w, x) \qquad f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

Optimization Definition

$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l \boxed{x_k x_l}$$

Constraints

$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$

Back to Primal

$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$

Predict

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$$f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k \boxed{x_k x})$$

Optimization Definition	$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l \, K(x_k x_l)$$
Constraints	$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$
Back to Primal	$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$
Predict	$$f(x,w) = sign(w,x) \qquad f(x,w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

Optimization Definition

$$max_{\alpha_k} \sum_{k=1}^{R} \alpha_k - \frac{1}{2} \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l y_k y_l \, K(x_k x_l)$$

Constraints

$$s.t \quad 0 \leq \alpha_k \leq C \quad \sum_{k=1}^{R} \alpha_k y_k = 0$$

We still need to compute all the kernels pairs, but we don't need to maintain the feature space

Back to Primal

$$w = \sum_{k=1}^{R} \alpha_k y_k x_k$$

Predict

$$f(x, w) = sign(w, x) \qquad f(x, w) = sign(\sum_{k=1}^{R} \alpha_k y_k x_k x)$$

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Good Kernel Functions for SVM

On top the polynomial kernel function there are more suitable ones:

Radial Basis Function (RBF):

$$K(X_i, X_j) = exp\left(-\frac{(X_i - X_j)^2}{2\sigma^2}\right)$$

Tanh Function (nn):

$$K(X_i, X_j) = tanh\left(\kappa X_i X_j - \delta\right)$$

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hypertune

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SVM Pros & Cons

Good

- Learn many non linear pattern
- Pick "conservative" hypotheses, that are less likely to overfit the data,
- Good for Small datasets with though target pattern
- “Only” 2 params - C, Kernel Function

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SVM Pros & Cons

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Bad

- O(n^2-3) runtime depends on C and the kernel (n number of datapoints)
- O(n^2) memory to compute all the pairwise kernels - 5-10K datapoints
- different values for the Kernel prams

Q&A

VC Dimension - https://www.youtube.com/watch?v=puDzy2XmR5c

https://winvector.github.io/margin/margin.pdf
https://youtu.be/LceLJvKMbBk?t=7311
https://youtu.be/fB47g3QM0sk?t=839

Shalev-Shwartz, S., Singer, Y., Srebro, N., & Cotter, A. (2011). Pegasos: Primal estimated sub-gradient solver for svm. Mathematical programming, 127(1), 3-30. [[pdf](http://www.ee.oulu.fi/research/imag/courses/Vedaldi/ShalevSiSr07.pdf)]

Schölkopf, B., Williamson, R. C., Smola, A. J., Shawe-Taylor, J., & Platt, J. C. (2000). Support vector method for novelty detection. In Advances in neural information processing systems (pp. 582-588). [[pdf](http://papers.nips.cc/paper/1723-support-vector-method-for-novelty-detection.pdf)]

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https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote09.html