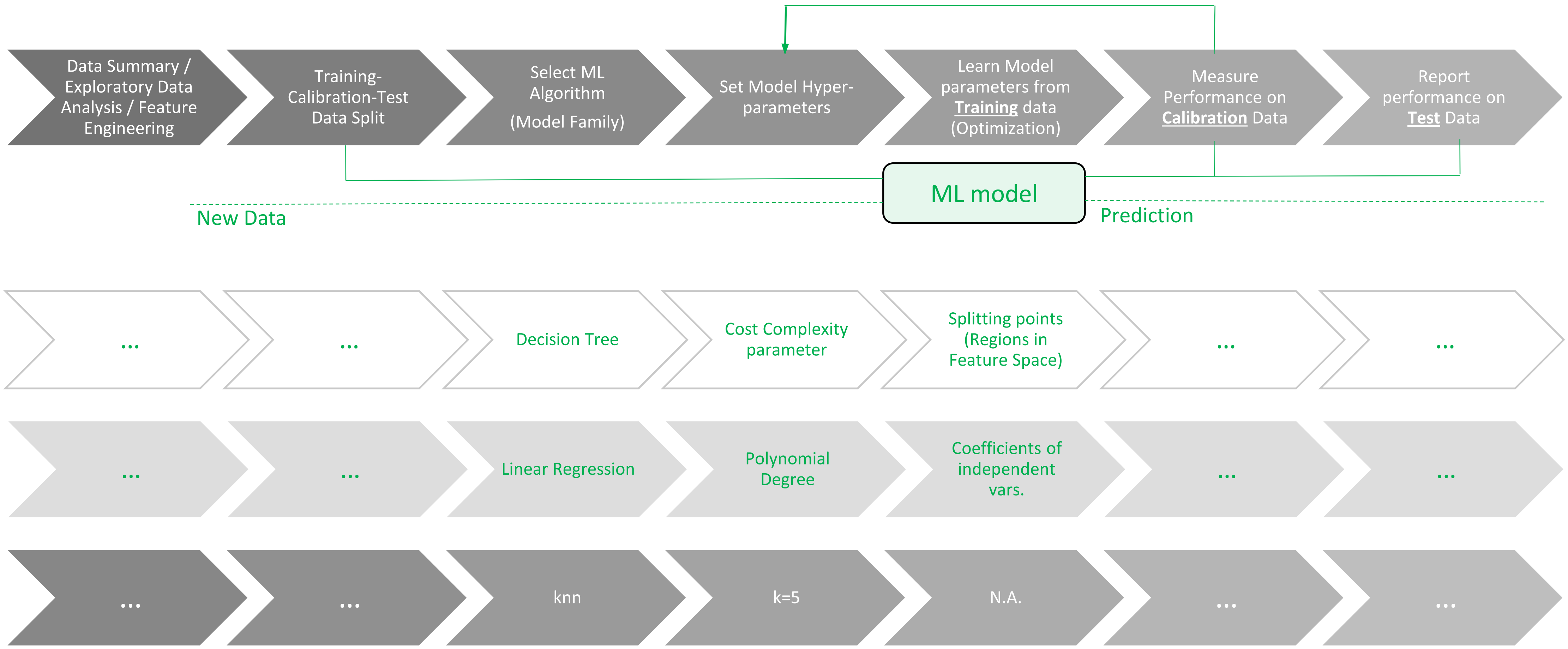
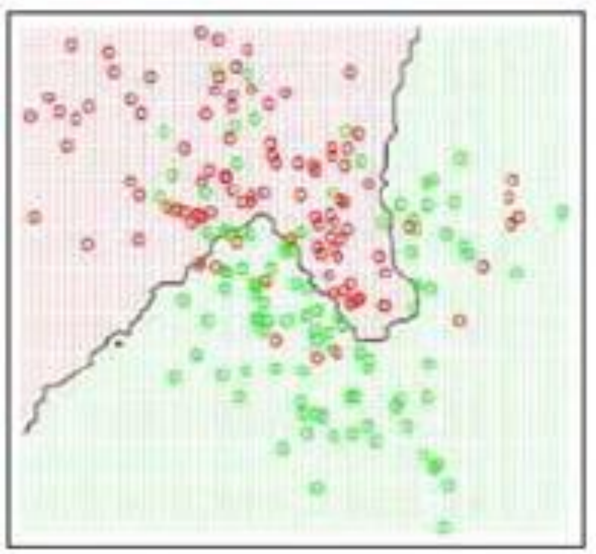
Support Vector Machines

Praphul Chandra

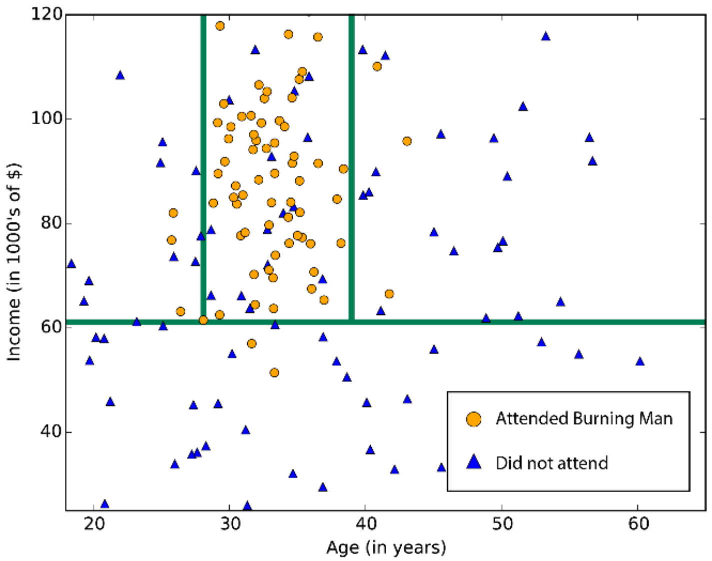
Machine Learning Framework



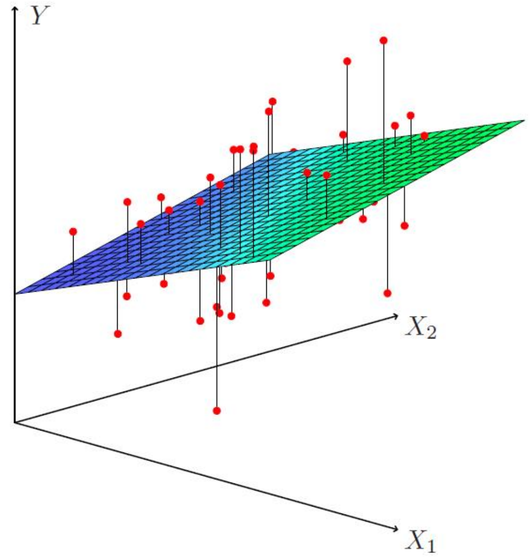
Classification vs. Regression *(p=2)*



knn



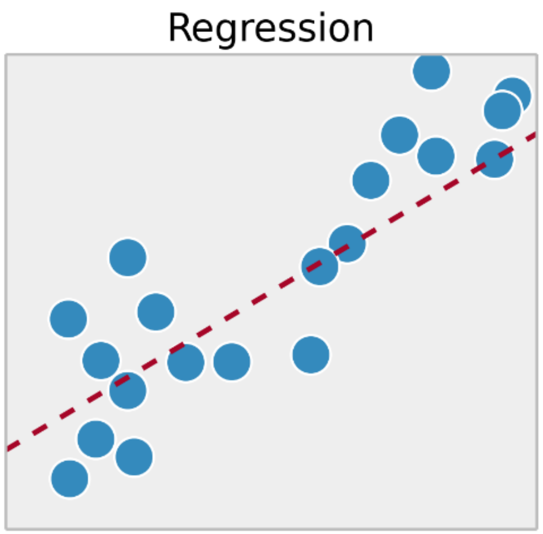
Decision Trees

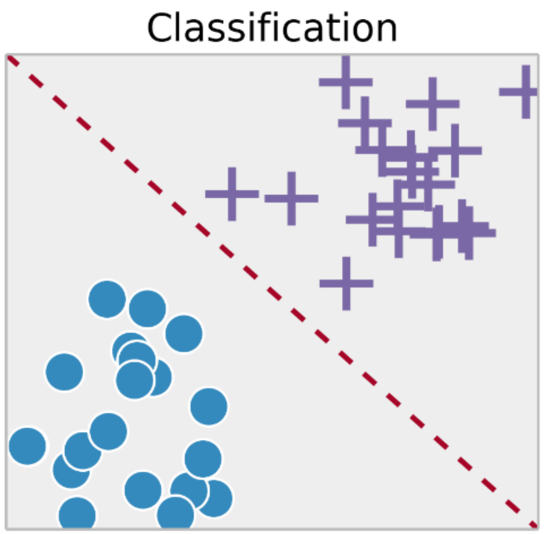


Linear Regression

- The lines / curves play a different role
  - Regression : approximate the mean value of the dependent variable given independent variables
  - Classification : separating boundary
- Different Algorithms / Model Families result in different curves / shapes
  - Model-Free
  - Locally Linear
  - Globally Linear

"Linear" Classification?





- Linear Regression
- Linear Classification ($y \in \{-1,1\}^n$)
  - Linear Separating Hyperplane

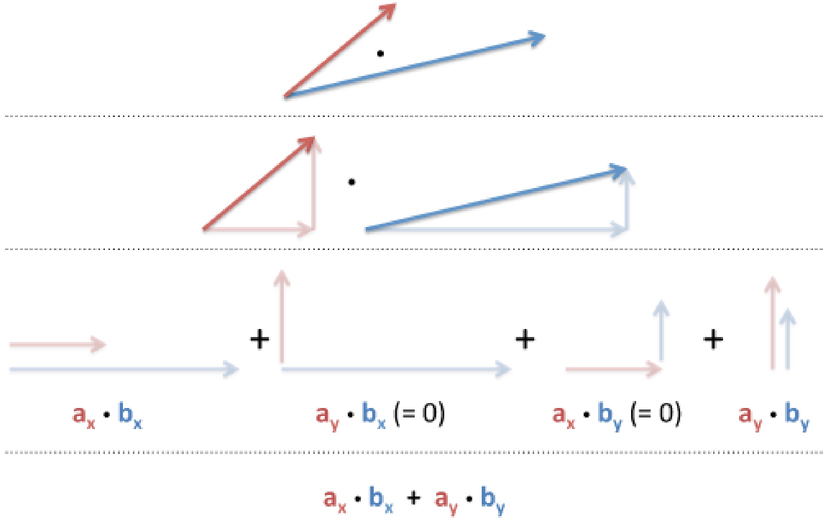
The Dot Product

- Inner Product
  - Element wise product of two vectors
  - a.k.a. scalar product

$$\begin{pmatrix} 3 \\ -2 \\ 6 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \\ -5 \end{pmatrix} = 3\times 2+(-2)\times 3+6\times(-5) = 6 - 6 - 30 = -30.$$

$$\mathbf{w} \in \mathbb{R}^p, \mathbf{x} \in \mathbb{R}^p$$

$$\mathbf{w}^T\mathbf{x} = \sum_{j=1}^{p} w_j x_j = \langle \mathbf{w}, \mathbf{x} \rangle$$

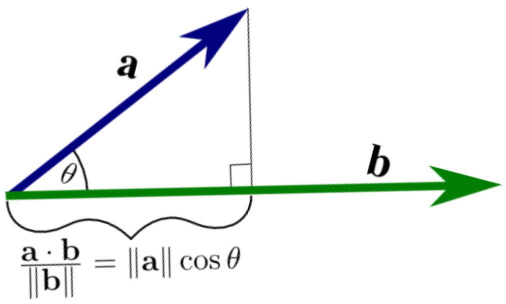


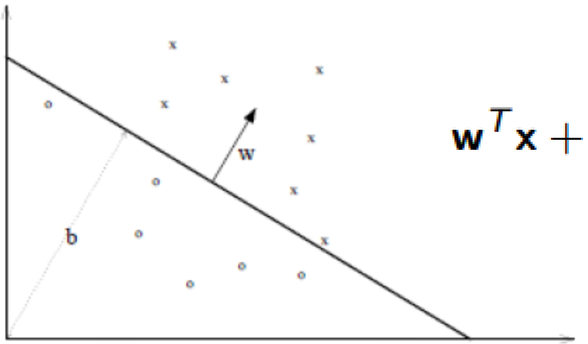
- Projection Product
  - Vector : Magnitude (Length) & Direction

$$\begin{aligned} \mathbf{w}^T\mathbf{x} &= ||\mathbf{w}||||\mathbf{x}|| \cos\theta \\ \theta = 90 &\Rightarrow \mathbf{w}^T\mathbf{x} = 0 \\ \theta = 0 &\Rightarrow \mathbf{w}^T\mathbf{x} = ||\mathbf{w}||||\mathbf{x}|| \\ \mathbf{w}^T\mathbf{w} &= ||\mathbf{w}||^2 \end{aligned}$$

$$\mathbf{x}_{\mathbf{w}} = ||\mathbf{x}|| \cos\theta = \frac{||\mathbf{x}||||\mathbf{w}|| \cos\theta}{||\mathbf{w}||} = \frac{\mathbf{x}^T\mathbf{w}}{||\mathbf{w}||} = \mathbf{x}^T\left(\frac{\mathbf{w}}{||\mathbf{w}||}\right) = \mathbf{x}^T\hat{\mathbf{w}}$$

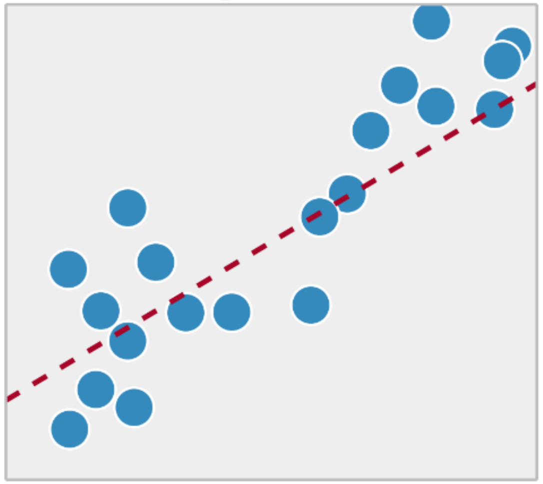
  - Equation of a hyperplane in p-dimensional space
  - Distance from origin, slope via orthogonal vector

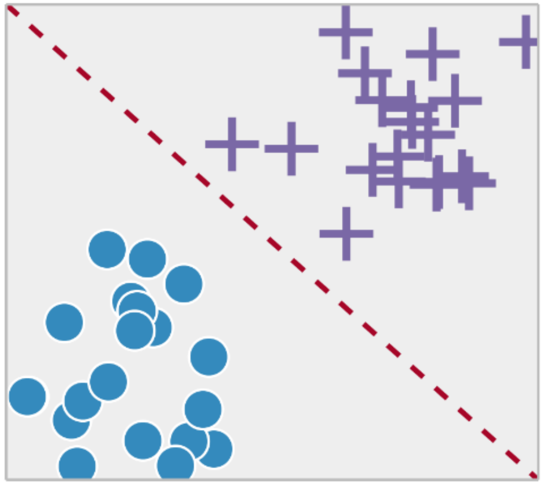




$$\mathbf{w}^T\mathbf{x} + b$$

"Linear" Classification?





- Linear Regression

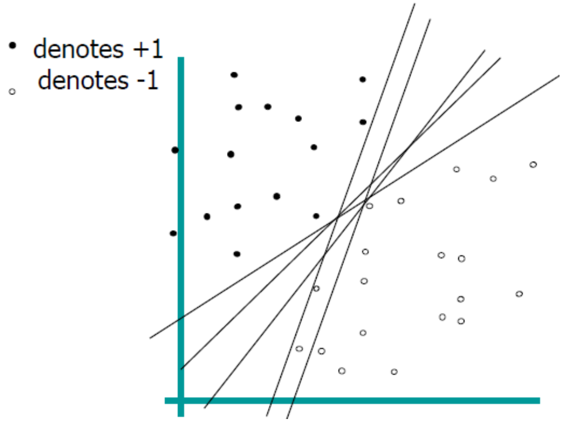
$$
\begin{aligned}
y_i, b \in \mathbb{R} \quad &, \quad \mathbf{x_i}, \mathbf{w} \in \mathbb{R}^p \\
&= \quad b + w_1 x_{i1} + w_2 x_{i2} + \ldots + w_p x_{ip} + \epsilon_i \\
&= \quad b + \sum_{j=1}^{p} w_j x_{ij} + \epsilon_i \\
&= \quad b + \mathbf{w}^T \mathbf{x_i} + \epsilon_i
\end{aligned}
$$

- Linear Classification ($y \in \{-1,1\}^n$)
  - Linear Separating Hyperplane

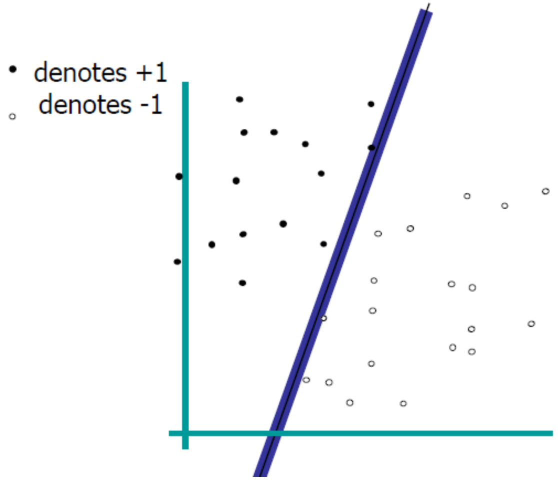
$$
\begin{aligned}
y_i \in \{-1, 1\}, b \in \mathbb{R} \quad &, \quad \mathbf{x_i}, \mathbf{w} \in \mathbb{R}^p \\
y_i \quad &= \quad \mathrm{sign}(b + \mathbf{w}^T \mathbf{x_i})
\end{aligned}
$$

Maximum Margin Classifier

- Many possible linear separating hyperplanes
  - Which one to choose?



- !dea
  - Margin of a classifier
  - Choose the linear classifier with the largest margin
  - Create the thickest hyper-slab which separates the two classes



- Optimization Criteria
  - Maximize the margin
  - subject to “training observations should lie on the correct side of the margin”
  - and “normalize coefficients” *(so that margins from hyperplanes are comparable)*

$$\min_{\mathbf{w}} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left(y_i - b - \mathbf{w}^T \mathbf{x_i} \right)^2$$

Linear Regression

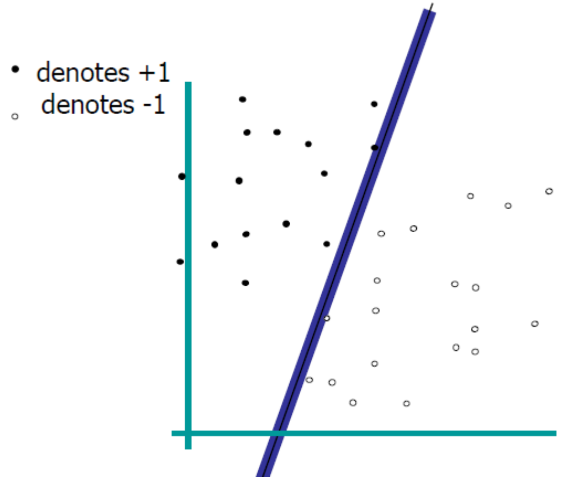
$$: \quad \max_{\mathbf{w}} M$$

$$\text{s.t.} \quad y_i(b + \mathbf{w}^T \mathbf{x_i}) > M \quad \forall i,$$

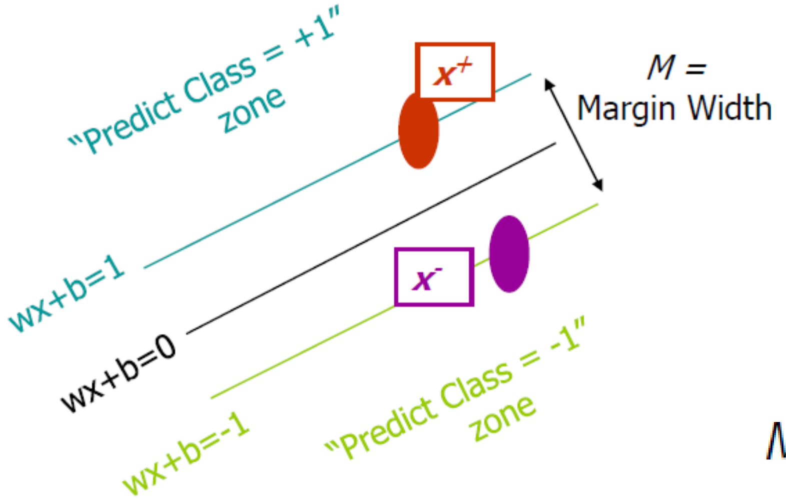
$$\text{and} \quad ||\mathbf{w}|| = \sum_{j=1}^{p} w_j^2 = 1$$

Maximum Margin Classification

Maximum Margin Classifier : Optimization revisited



- Setup : ($y_i \in \{-1,1\}$)
  - x^+: Nearest positive class training observation closest to the separating hyperplane
  - x^-: Nearest negative class training observation closest to the separating hyperplane



$$
\begin{aligned}
b + \mathbf{w}^T \mathbf{x}^+ &= +1 \\
b + \mathbf{w}^T \mathbf{x}^- &= -1 \\
\mathbf{w}^T (\mathbf{x}^+ - \mathbf{x}^-) &= 2
\end{aligned}
$$

$$
M = \frac{\mathbf{w}}{||\mathbf{w}||} \cdot (\mathbf{x}^+ - \mathbf{x}^-) = \frac{2}{||\mathbf{w}||}
$$

- Margin
  - Projection of $(x^+ - x^-)$ onto the unit vector normal to the separating hyperplane

$$
\begin{aligned}
: \quad & \max_{\mathbf{w}} M \\
\text{s.t.} \quad & y_i(b + \mathbf{w}^T \mathbf{x_i}) > M \quad \forall i, \\
\text{and} \quad & ||\mathbf{w}|| = \sum_{j=1}^{p} w_j^2 = 1
\end{aligned}
$$

- Equivalent Optimization Problem
  - Minimize hyperplane parameters ~ Maximize Margin

$$
\begin{aligned}
: \quad & \min \mathbf{w}^T \mathbf{w} \\
\text{s.t.} \quad & y_i(b + \mathbf{w}^T \mathbf{x_i}) > 0 \quad \forall i
\end{aligned}
$$

Support Vector Classifier

$$
\begin{aligned}
y_i, b \in \mathbb{R} \quad &, \quad \mathbf{x_i}, \mathbf{w} \in \mathbb{R}^p \\
&= b + w_1 x_{i1} + w_2 x_{i2} + \ldots + w_p x_{ip} + \epsilon_i \\
&= b + \sum_{j=1}^{p} w_j x_{ij} + \epsilon_i \\
&= b + \mathbf{w}^T \mathbf{x_i} + \epsilon_i
\end{aligned}
$$

$$
\begin{aligned}
y_i \in \{-1, 1\}, b \in \mathbb{R} \quad &, \quad \mathbf{x_i}, \mathbf{w} \in \mathbb{R}^p \\
y_i \quad &= \quad \text{sign}(b + \mathbf{w}^T \mathbf{x_i})
\end{aligned}
$$

- Motivation
  - A change of one observation result in a significant change in the hyperplane
  - Maximum Margin classifier has high variance

- !dea
  - Add some slack
  - Hyper-parameter : Total slack allowed

$$
\begin{aligned}
: \quad & \max_{\mathbf{w},\epsilon} M \\
\text{s.t.} \quad & y_i(b + \mathbf{w}^T \mathbf{x_i}) > M(1 - \epsilon_i) \quad \forall i. \\
\text{and} \quad & \sum_{j=1}^{n} \epsilon_i \leq C \\
\text{and} \quad & ||\mathbf{w}|| = 1
\end{aligned}
$$

- Support Vector (a.k.a. Soft Margin) Classifier
  - Margin is “soft” i.e. allows some training observations to lie on the wrong side of the margin / hyperplane

Maximum Margin Classifier : Optimization revisited : again

- Yet another (optimization) equivalence
  - Primal - Dual
  - Solving the Dual involves computing only *dot products* among all training points
  - $\alpha_i \neq 0$ ➔ x_i is a **support vector**

- The classification function depends only on the *dot product* of the test observation with **support vectors.**

- Intuition
  - The hyperplane is “supported” by the training data observations which are closest to it
  - The margin depends on how close (near) the support vectors from two classes are to each other

$$: \quad \max_{\mathbf{w}} M$$
$$\text{s.t.} \quad y_i(b + \mathbf{w}^T\mathbf{x_i}) > M \quad \forall i,$$
$$\text{and} \quad ||\mathbf{w}|| = \sum_{j=1}^{p} w_j^2 = 1$$

$$: \quad \min \mathbf{w}^T\mathbf{w}$$
$$\text{s.t.} \quad y_i(b + \mathbf{w}^T\mathbf{x_i}) > 0 \quad \forall i$$

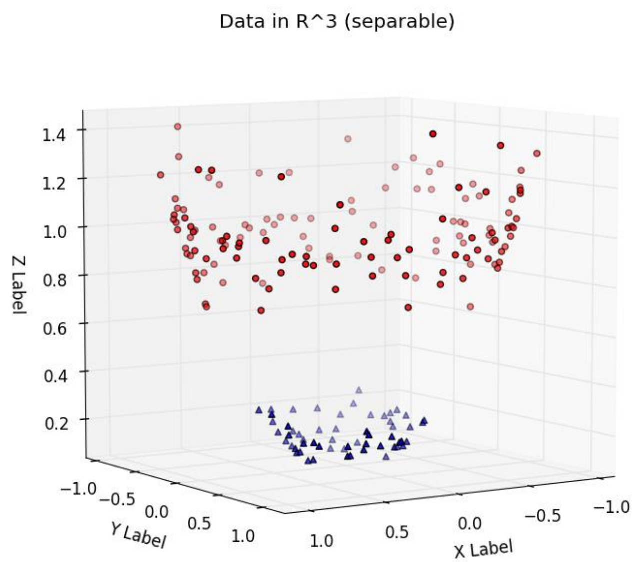
$$: \quad \max_{\alpha} \left(\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x_i}^T \mathbf{x_j} \right)$$
$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \quad \forall i$$
$$\text{and} \quad \alpha_i \geq 0 \quad \forall i$$

Solution to the dual : $\alpha \in \mathbb{R}^n$ means

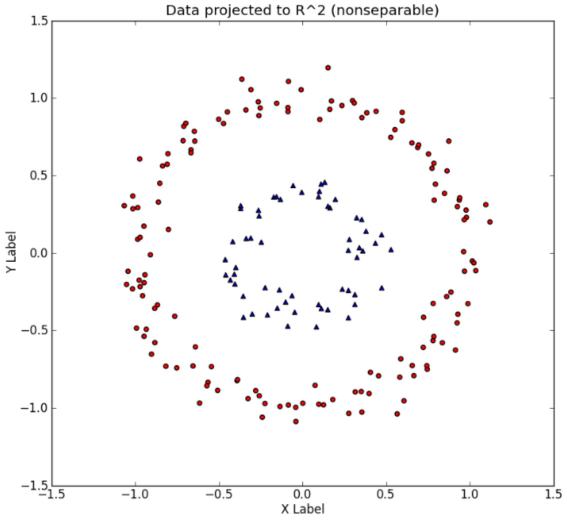
$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$
$$b = y_k - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^T \mathbf{x_k} \quad \text{for any} k$$
$$f(\mathbf{x}^*) = \mathbf{w}^T\mathbf{x}^* + b = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^T \mathbf{x}^* + b$$

Support Vector Machine

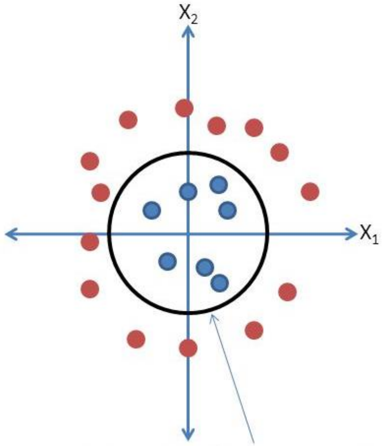
- Motivation
  - Is a “linear” separating hyperplane always possible?
  - Even with the slack?



- !ntuition
  - Data which is <u>separable</u> with a linear hyperplane may not be linearly separable in a **lower** dimension sub-space
  - Data which is <u>not separable</u> with a linear hyperplane may be linearly separable in a **higher** dimension space
  - Can we increase the dimensionality of the data and then linearly separate it?
  - How?
  - At what cost?



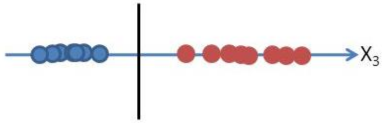
Achieving Non-Linearity using Dimensionality Expansion



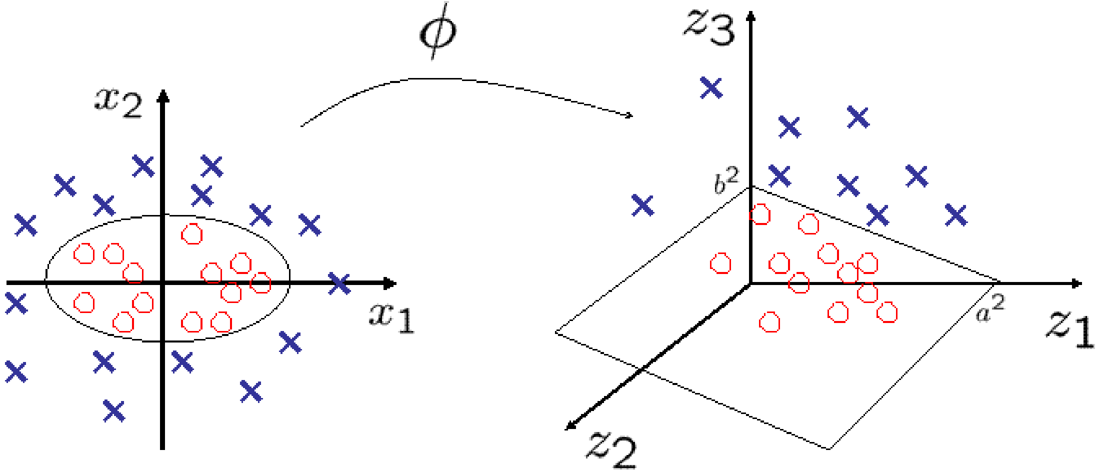
In the original feature space, the linear separator looks like a circle.

The Kernel Trick is to add a new input variable that is computed from the existing ones.

Let $X_3 = \sqrt{X_1^2 + X_2^2}$



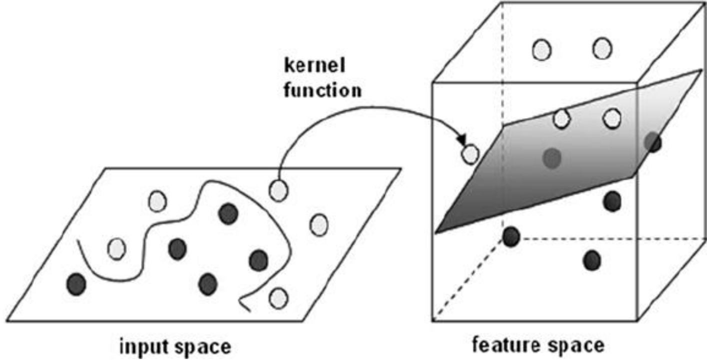
Now there's a linear separator!



$$\phi : (x_1, x_2) \longrightarrow (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

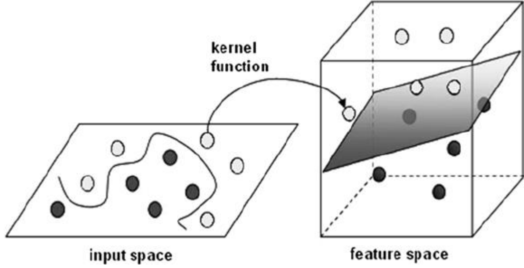
$$\left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b}\right)^2 = 1 \longrightarrow \frac{z_1}{a^2} + \frac{z_3}{b^2} = 1$$

Dimension Expansion to tackle Non-Linearity



- The curse of dimensionality
  - Exponential increase in volume associated with adding extra dim *(e.g. Impact on knn)*
  - With a fixed number of training samples, predictive power reduces as the dimensionality increases *(Hughes effect)*
  - Computational Complexity
  - Dimensionality reduction techniques: Principal Component Analysis
- The boon of dimensionality
  - Data which is not linearly separable in m-dimensions may be separable in m+ dimensions
  - Used beyond SVM : Polynomial regression, Basis Transformation
- The beauty of SVM
  - Achieve benefits of dimensionality expansion (linear separability) without paying the computational cost
  - The solution to the optimization problem requires us to calculate ONLY the **dot product** among the support vectors
  - Define a kernel function corresponding to the generalization of the **dot product** *(Reduced computational cost)*
  - Define a kernel function which captures the proximity of the support vectors *(Further Reduced computational cost)*

The Kernel Trick : Dot Product Magic



$$\Phi(\mathbf{x}) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \vdots \\ \sqrt{2}x_m \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_m^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \sqrt{2}x_2x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \vdots \\ \sqrt{2}x_{m-1}x_m \end{pmatrix}$$

Constant Term

Linear Terms

Pure Quadratic Terms

Quadratic Cross-Terms

$$\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) = \begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ \vdots \\ \sqrt{2}a_m \\ a_1^2 \\ a_2^2 \\ \vdots \\ a_m^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \sqrt{2}a_2a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \vdots \\ \sqrt{2}a_{m-1}a_m \end{pmatrix} \bullet \begin{pmatrix} 1 \\ \sqrt{2}b_1 \\ \sqrt{2}b_2 \\ \vdots \\ \sqrt{2}b_m \\ b_1^2 \\ b_2^2 \\ \vdots \\ b_m^2 \\ \sqrt{2}b_1b_2 \\ \sqrt{2}b_1b_3 \\ \vdots \\ \sqrt{2}b_1b_m \\ \sqrt{2}b_2b_3 \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \sqrt{2}b_{m-1}b_m \end{pmatrix}$$

$$1 + \sum_{i=1}^{m} 2a_ib_i + \sum_{i=1}^{m} a_i^2b_i^2 + \sum_{i=1}^{m}\sum_{j=i+1}^{m} 2a_ia_jb_ib_j$$

Computational Cost

$O(m^2)$ for quadratic expansion

$O(m^d)$ in general

Define K(**a**,**b**) = $(\mathbf{a}.\mathbf{b}+1)^2$

$$= (\mathbf{a}.\mathbf{b})^2 + 2\mathbf{a}.\mathbf{b} + 1$$

$$= \left(\sum_{i=1}^{m} a_ib_i\right)^2 + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m}(a_ib_i)^2 + 2\sum_{i=1}^{m}\sum_{j=i+1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

Computational Cost

O(m)

$$K_{\text{linear}}(\mathbf{a},\mathbf{b}) = \mathbf{a}^T\mathbf{b}$$

$$K_{\text{polynomial}}(\mathbf{a},\mathbf{b}) = (\mathbf{a}^T\mathbf{b}+1)^d$$

$$K_{\text{rbf}}(\mathbf{a},\mathbf{b}) = \exp\left(-\frac{||\mathbf{a}-\mathbf{b}||^2}{2\sigma^2}\right)$$

$$K_{\text{tanh}}(\mathbf{a},\mathbf{b}) = \tanh(\kappa\mathbf{a}^T\mathbf{b}-\delta)$$

Support Vector Machine : Summary

- !deas
  1) Linear Separating Hyperplane
  2) Add slack to reduce variance
  3) Achieve benefits of dimensionality expansion (linear separability) without paying the computational cost
     - The solution to the optimization problem requires us to calculate ONLY the **dot product** among the support vectors
     - Define a kernel function corresponding to the generalization of the **dot product** *(Reduced computational cost)*
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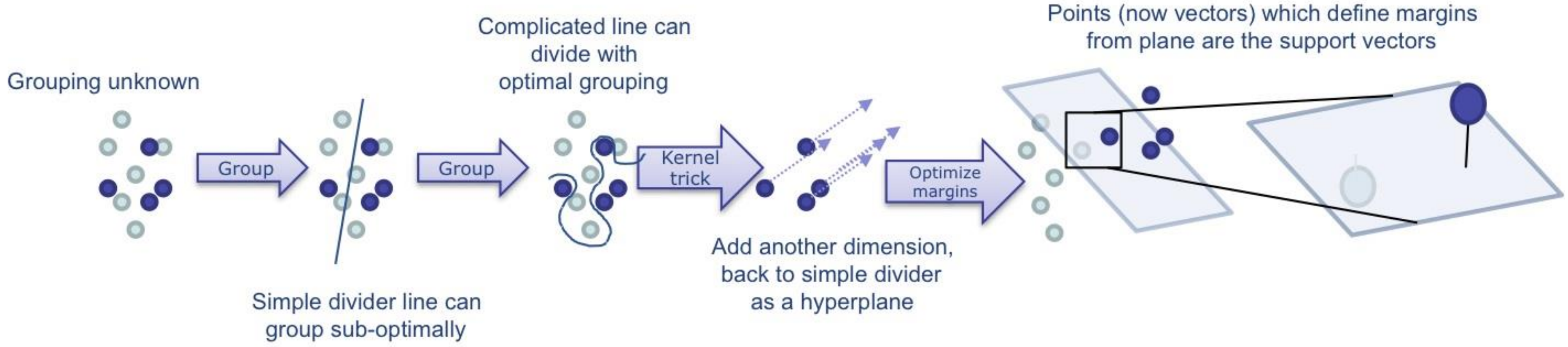
- Hyperparameters
  - Choice of Kernel : Linear / Polynomial / Radial Basis Function
  - Total Slack (softness) allowed



Using SVMs

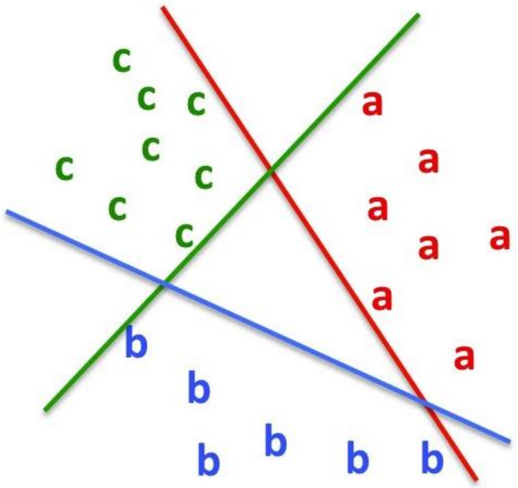
- Tuning SVM
  - Feature Engineering: Normalization, Scaling,
  - Hyperparameter: Use Cross Validation to find the best kernel family and kernel parameters

- Advantages
  - Flexible : different kernels try different "non-linear" boundaries (in the native feature space)
  - Exploits sparseness : use the support vectors only for determining the separating hyperplane
  - Can handle large feature spaces efficiently (computational complexity does not depend on p)
  - Good theoretical guarantees (Maximum margin generalizes better, Convex optimization guaranteed to converge)

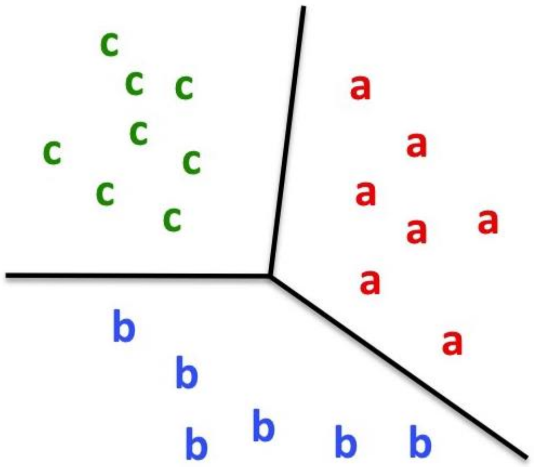
- Limitations
  - Sensitive to noise and outliers (Increasing the margin may reduce the accuracy)
  - Doesn't provide a posterior probability
  - Messy Multi-labelled classification (m-classes)
    - Train m 1-vs-Rest Binary classifiers (But this results in class imbalance – May require fine tuning of cost function)
    - Train Binary classifiers for m(m-1)/2 pairs of classes & classify based on which class receives highest votes (More computation)

Multi Class Classification as Binary Classification

- One vs. All
  - Train m Binary classifiers : One classifier per class
  - Base classifiers to produce a real-valued confidence score for its decision (SVM?)
  - a.k.a. One vs. Rest
  - Gotcha: May result in class imbalance



- One vs. One
  - Train m(m-1)/2 binary classifiers : One classifier per pair of classes
  - Classify a new sample based on which class receives highest votes
  - Gotcha: More computation!



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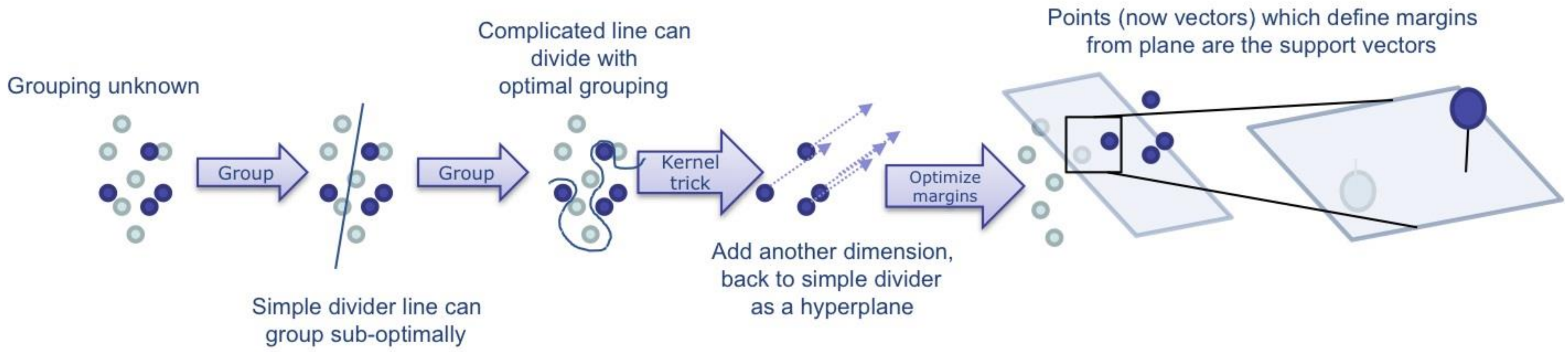
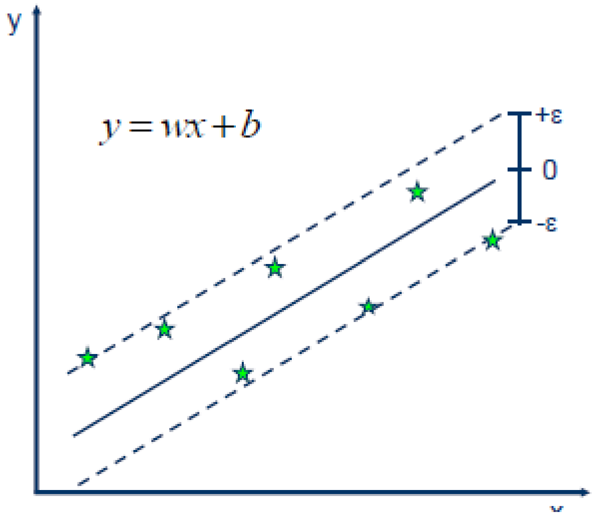


Before we finish … Support Vector Regression

- Regression extension
  - Modify the optimization problem
  - Want the hyperplane close to the “support” vectors
  - Reinterpret Slack

- Exploit the kernel trick
  - Linearity in high dimensions ➔ non-linearity in lower dimensions
  - Without the computational cost

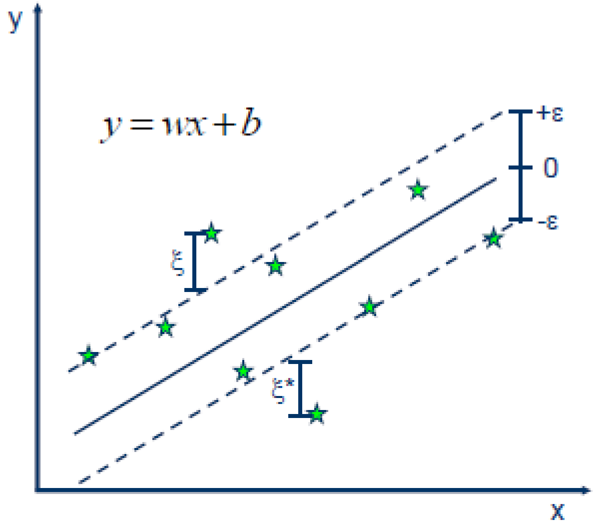


- Solution:

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

- Constraints:

$$y_i - wx_i - b \le \varepsilon$$
$$wx_i + b - y_i \le \varepsilon$$



- Minimize:

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\left(\xi_i + \xi_i^*\right)$$

- Constraints:

$$y_i - wx_i - b \le \varepsilon + \xi_i$$
$$wx_i + b - y_i \le \varepsilon + \xi_i^*$$
$$\xi_i, \xi_i^* \ge 0$$

Q?

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