Machine Learning, Spring 2019

Support Vector Machine

Reading Assignment: Chapter 5 & 6

Python tutorial: http://learnpython.org/

TensorFlow tutorial: https://www.tensorflow.org/tutorials/

PyTorch tutorial: https://pytorch.org/tutorials/

Acknowledge: The slides are partially referred to coursera online machine learning course by Prof. Andrew Ng, and NYU machine learning course. All copyrights owned by original authors.

Support Vector Machines (SVMs)

Support vector machines are an optimization based prediction approach used primarily for **binary classification**, and are able to achieve state-of-the-art prediction accuracy on many real-world tasks.

Key idea 1: Learn a **decision boundary** that optimally separates positive and negative training examples. (But what does it mean to be optimal?)

Key idea 2: Learn a **linear** decision boundary in high dimensional space corresponding to a **non-linear** decision boundary for the original problem.

SVM assumes **real-valued** attributes on the **same scale**. Thus it is very important to pre-process your data before training the model:

- Normalize real-valued attributes (scale either to [0,1] or to mean = 0 and variance = 1). Make sure to use same scaling for training and test data.
- Replace discrete-valued attributes with **dummy variables**.

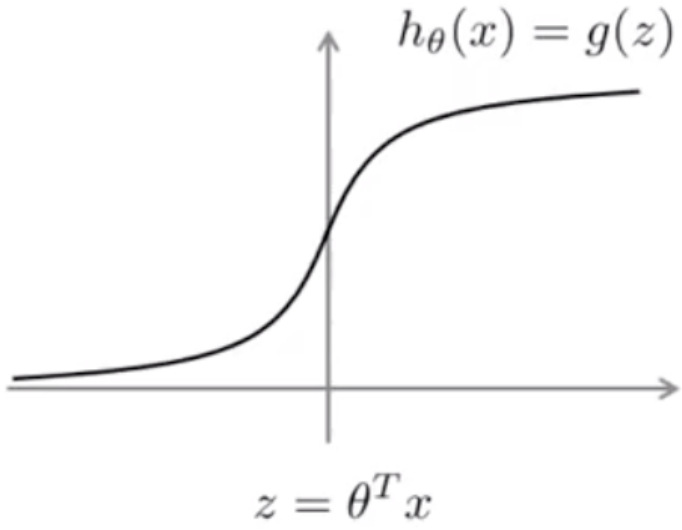
Car	Weight
1	Low
2	Medium
3	Heavy

⇨

Car	Weight=Medium	Weight=Heavy
1	0	0
2	1	0
3	0	1

From Logistic Regression to SVM

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$



If y =1, we wish our predicted hypothesis value is close to 1, then $\theta^T x \gg 0$

If y =0, we wish our predicted hypothesis value is close to 1, then $\theta^T x \ll 0$

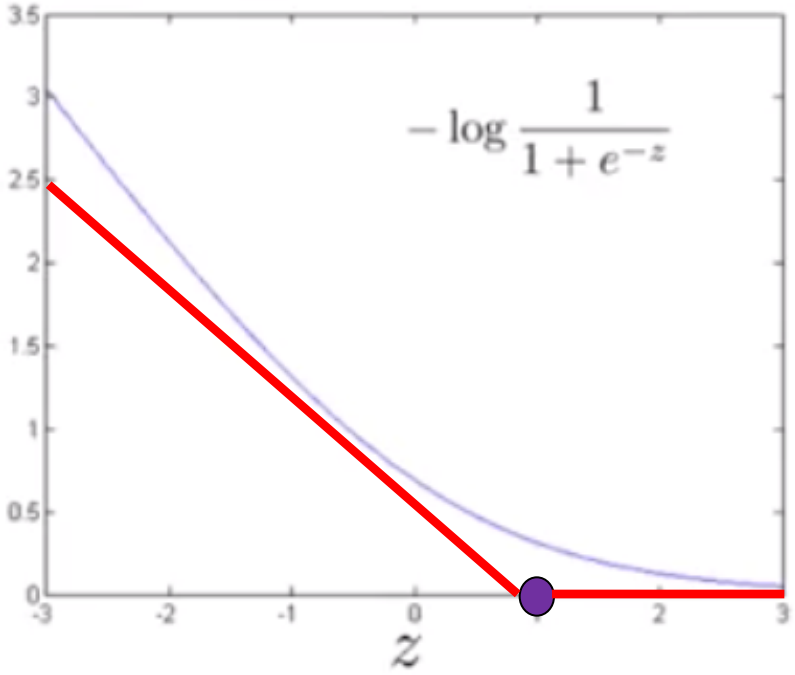
Cost function of Logistic Regression

Cost Function:

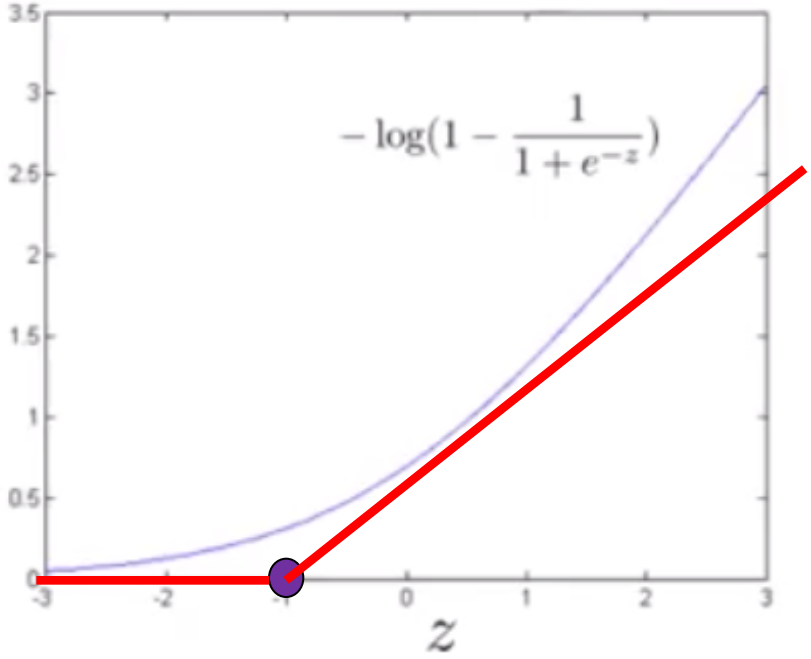
$$-(y \log h_\theta(x) + (1-y) \log(1 - h_\theta(x)))$$

$$= -y \log \frac{1}{1+e^{-\theta^T x}} - (1-y) \log(1 - \frac{1}{1+e^{-\theta^T x}})$$

y = 1

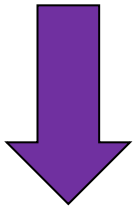

$-\log \frac{1}{1+e^{-z}}$
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2
-1
0
2
3
z

y = 0


$-\log(1-\frac{1}{1+e^{-z}})$
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2
0
1
2
3
z

Logistic regression:

$$\min_{\theta} \frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)}\left(-\log h_\theta(x^{(i)})\right) + (1-y^{(i)})\left(\left(-\log(1-h_\theta(x^{(i)}))\right)\right]+\frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$



Support vector machine:

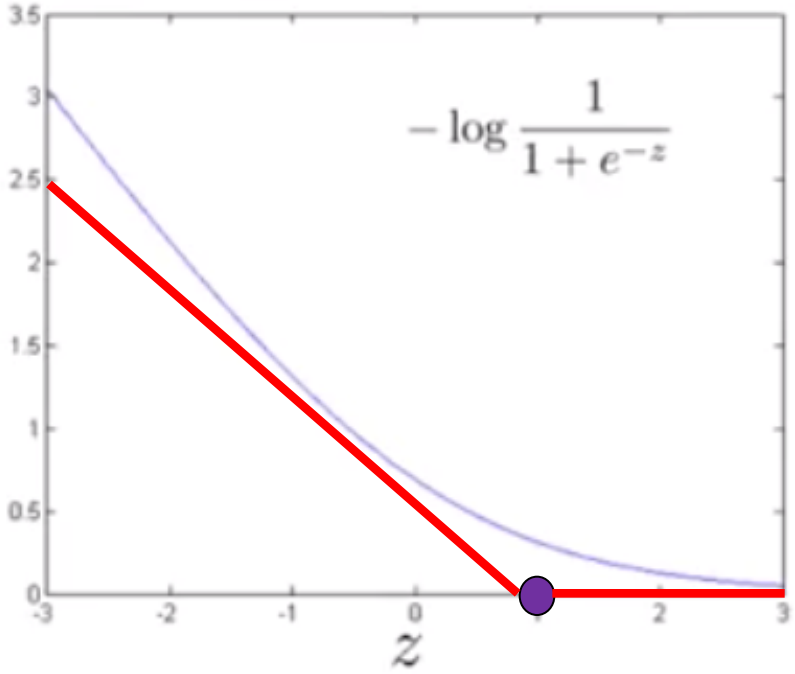
$$\min_{\theta} C\sum_{i=1}^{m}\left[y^{(i)}cost_1(\theta^T x^{(i)}) + (1-y^{(i)})cost_0(\theta^T x^{(i)})\right] + \frac{1}{2}\sum_{i=1}^{n}\theta_j^2$$

SVM Hypothesis

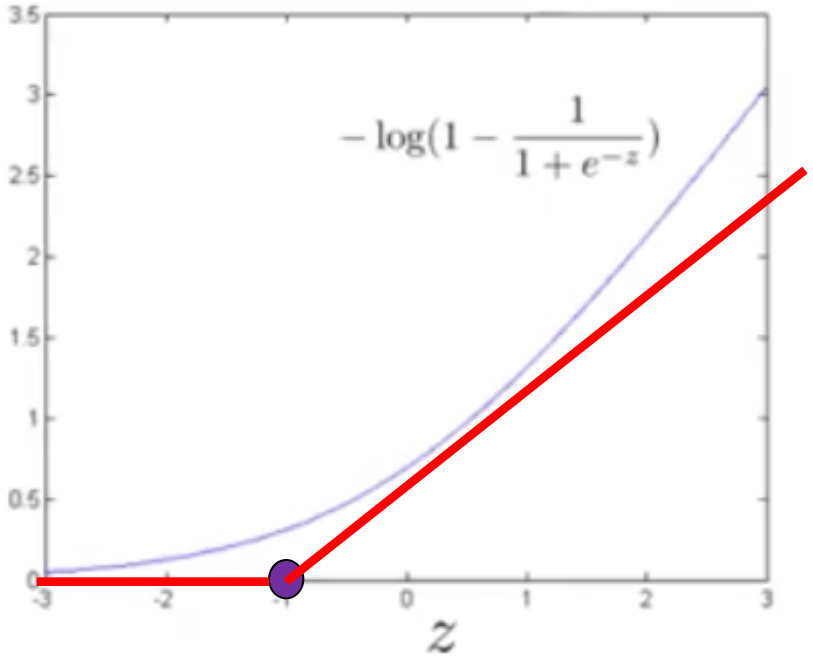
Support Vector Machine

$$\min_{\theta} C \sum_{i=1}^{m} \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T x^{(i)}) \right] + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

y = 1



y = 0



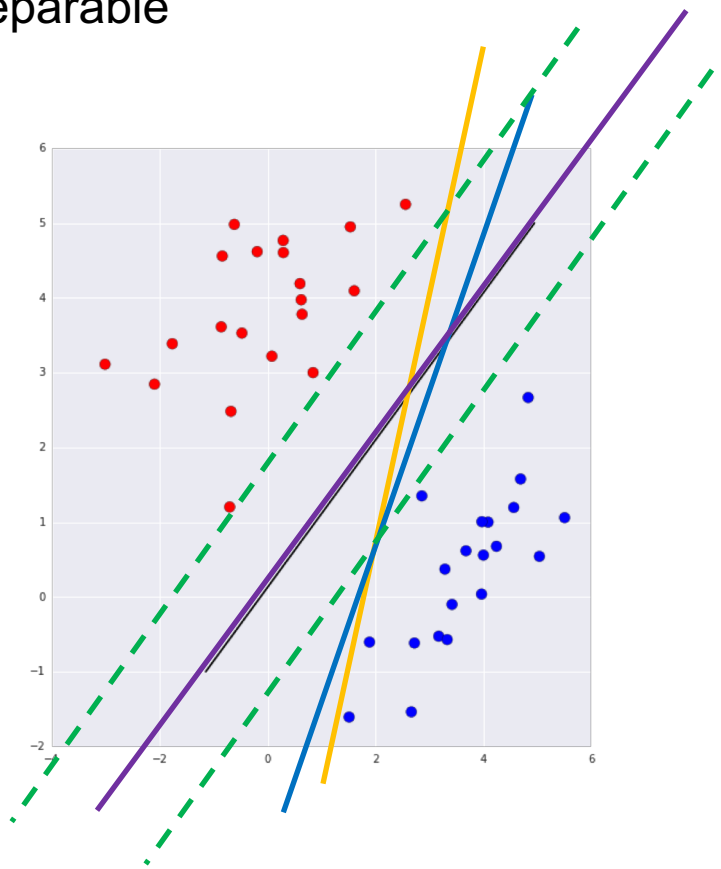
SVM Decision Boundary

$$\min_{\theta} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

$$\text{s.t.} \quad \theta^T x^{(i)} \geq 1 \qquad \text{if } y^{(i)} = 1$$

$$\theta^T x^{(i)} \leq -1 \qquad \text{if } y^{(i)} = 0$$

Example of linearly separable



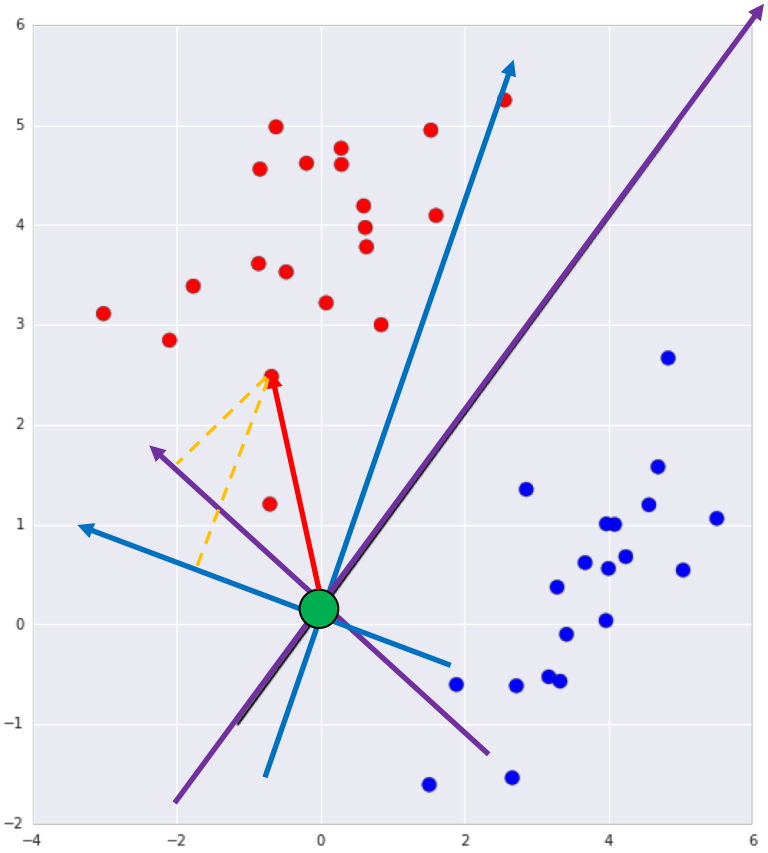
Large Margin Classifier

Why large margin works?

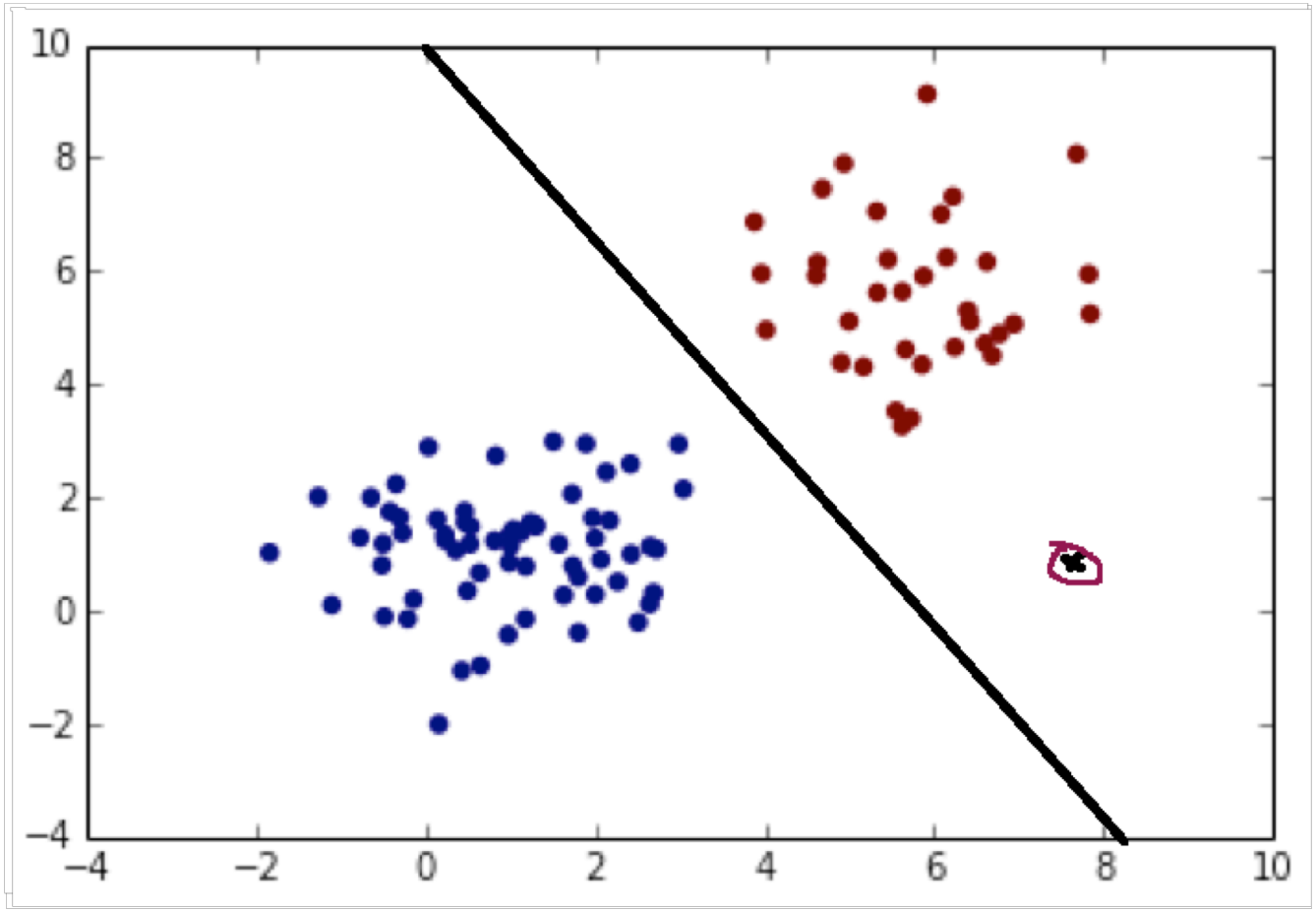
$$\min_{\theta} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

$$\text{s.t.} \quad \theta^T x^{(i)} \geq 1 \qquad \text{if } y^{(i)} = 1$$

$$\theta^T x^{(i)} \leq -1 \qquad \text{if } y^{(i)} = 0$$

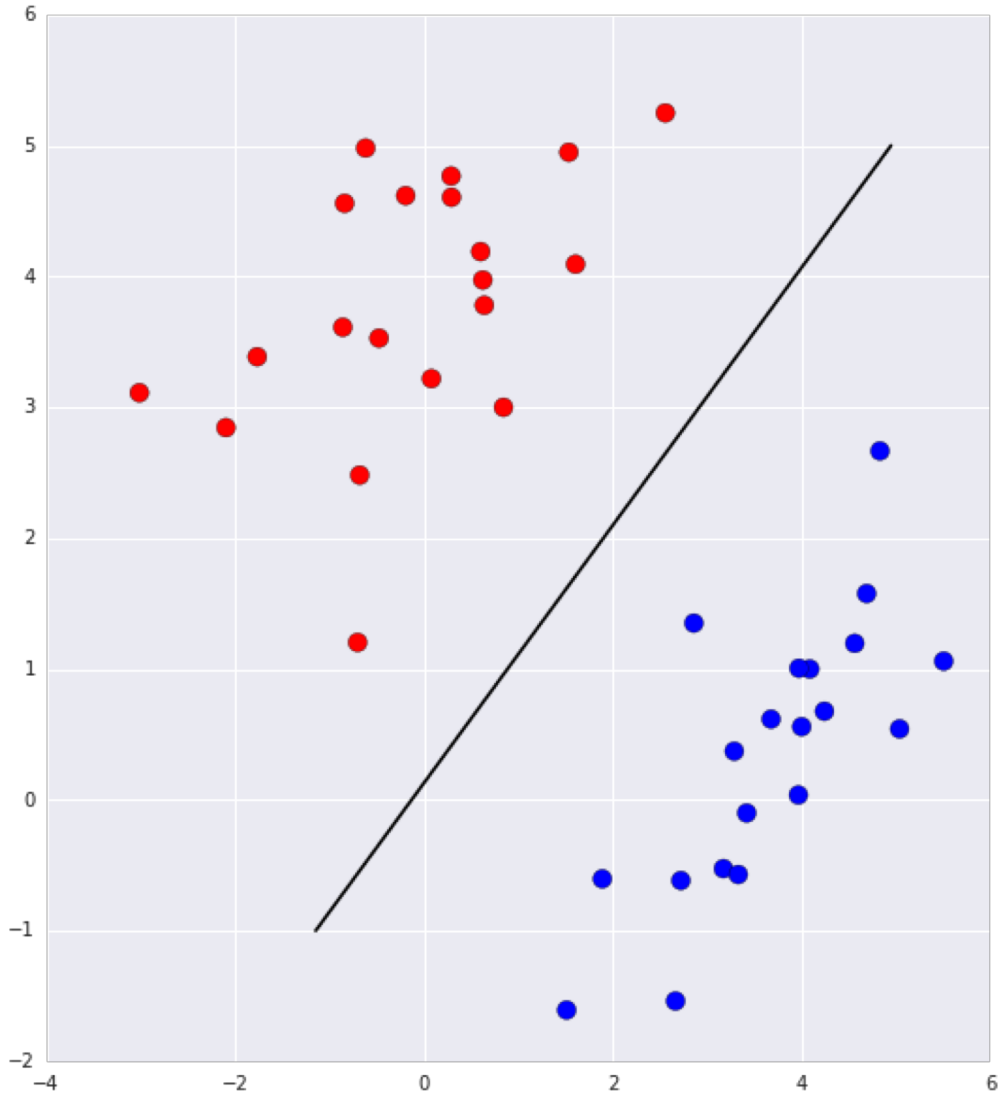


SVMs: the basic idea (linearly separable case)



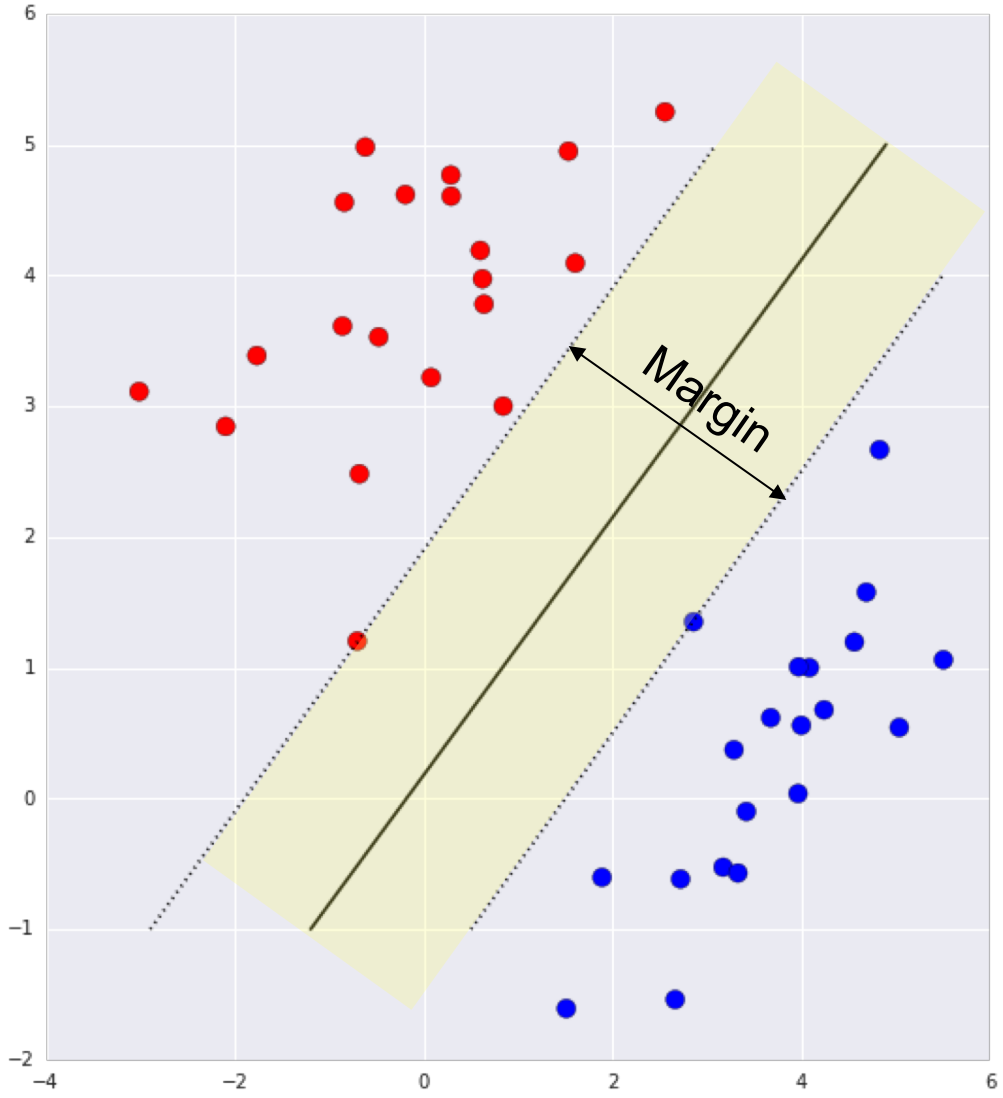
Which line to choose?

This is an optimization problem.



Which line to choose?

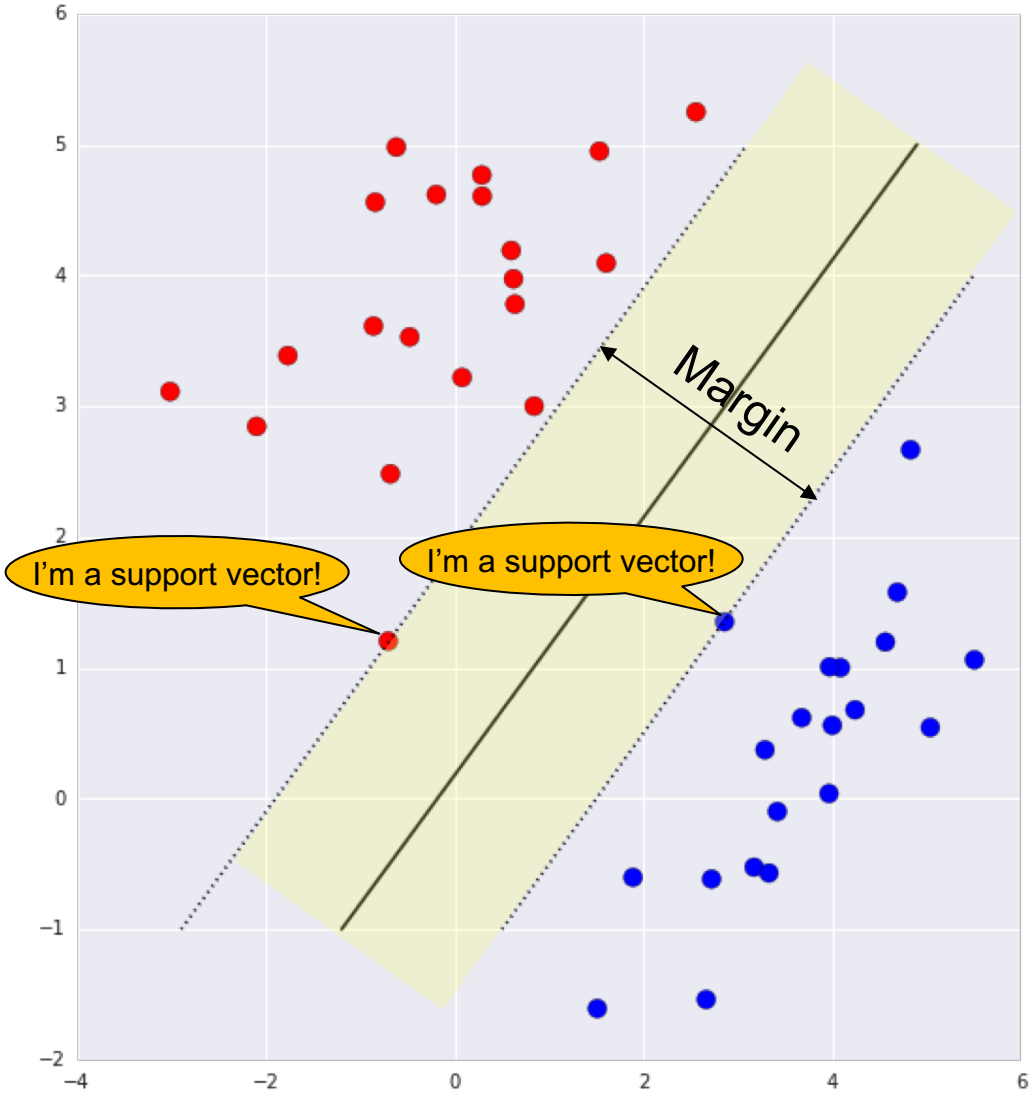
Choose the line that maximizes the **margin** between classes.



Margin = how **wide** we could make the linear decision boundary before it contacts points from either class.

Which line to choose?

Choose the line that maximizes the **margin** between classes.



Points on the margin are called **support vectors**.

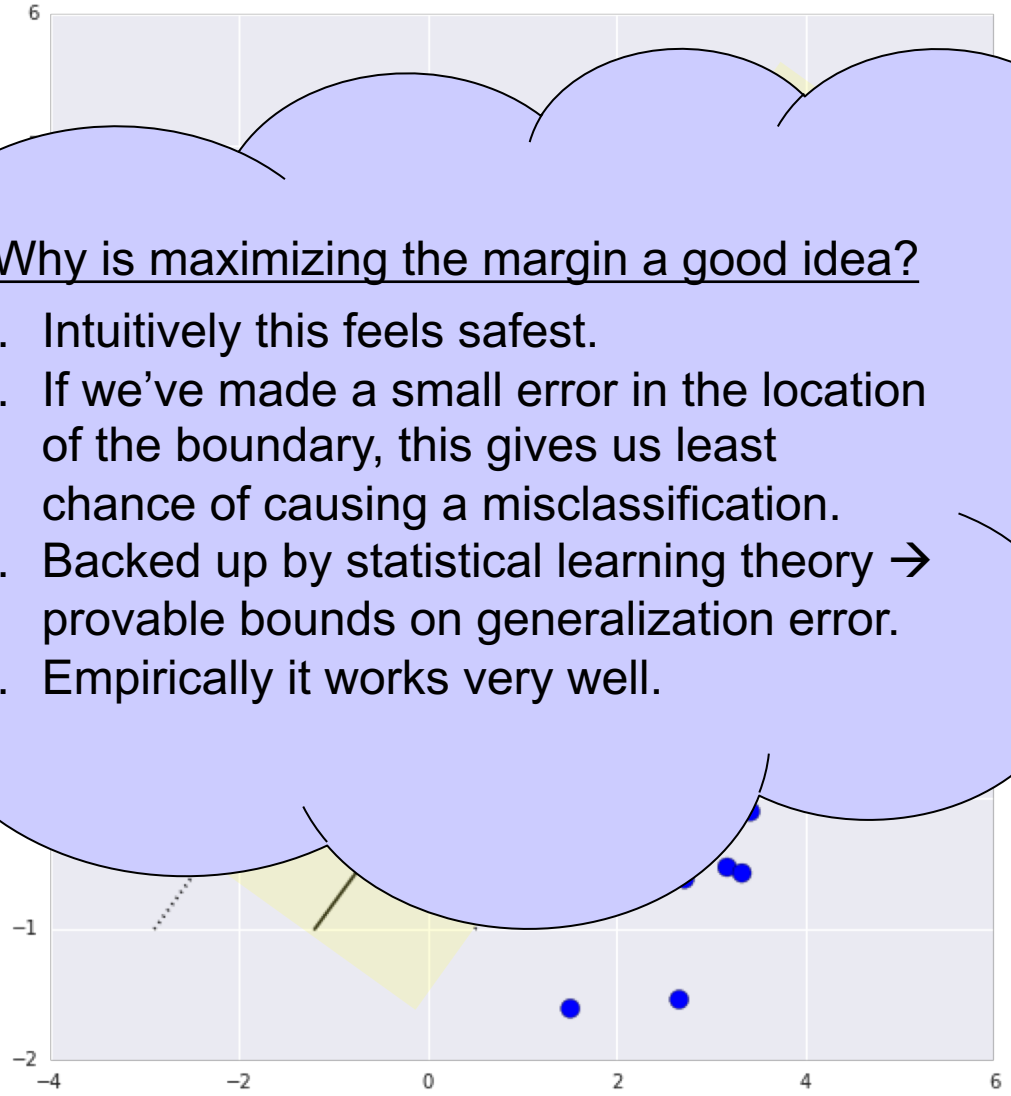
The classifier can be defined entirely by the set of support vectors.

This fact has lots of useful implications:

- Fast classification of test points.
- Fast leave-one-out cross-validation.
- Faster, but still expensive, training.

Which line to choose?

Choose the line that maximizes the **margin** between classes.



Why is maximizing the margin a good idea?

1. Intuitively this feels safest.
2. If we've made a small error in the location of the boundary, this gives us least chance of causing a misclassification.
3. Backed up by statistical learning theory → provable bounds on generalization error.
4. Empirically it works very well.

Points on the
argin are called
port vectors.

er can be
ely by the
rt vectors.

lots of
ations:

ification
oints.
ast leave-one-out
cross-validation.
Faster, but still
expensive, training.

How to maximize the margin?

To separate, for all points j, we must have:

$$y_j(x_j^T w + b) > 0$$

For the margin, define:

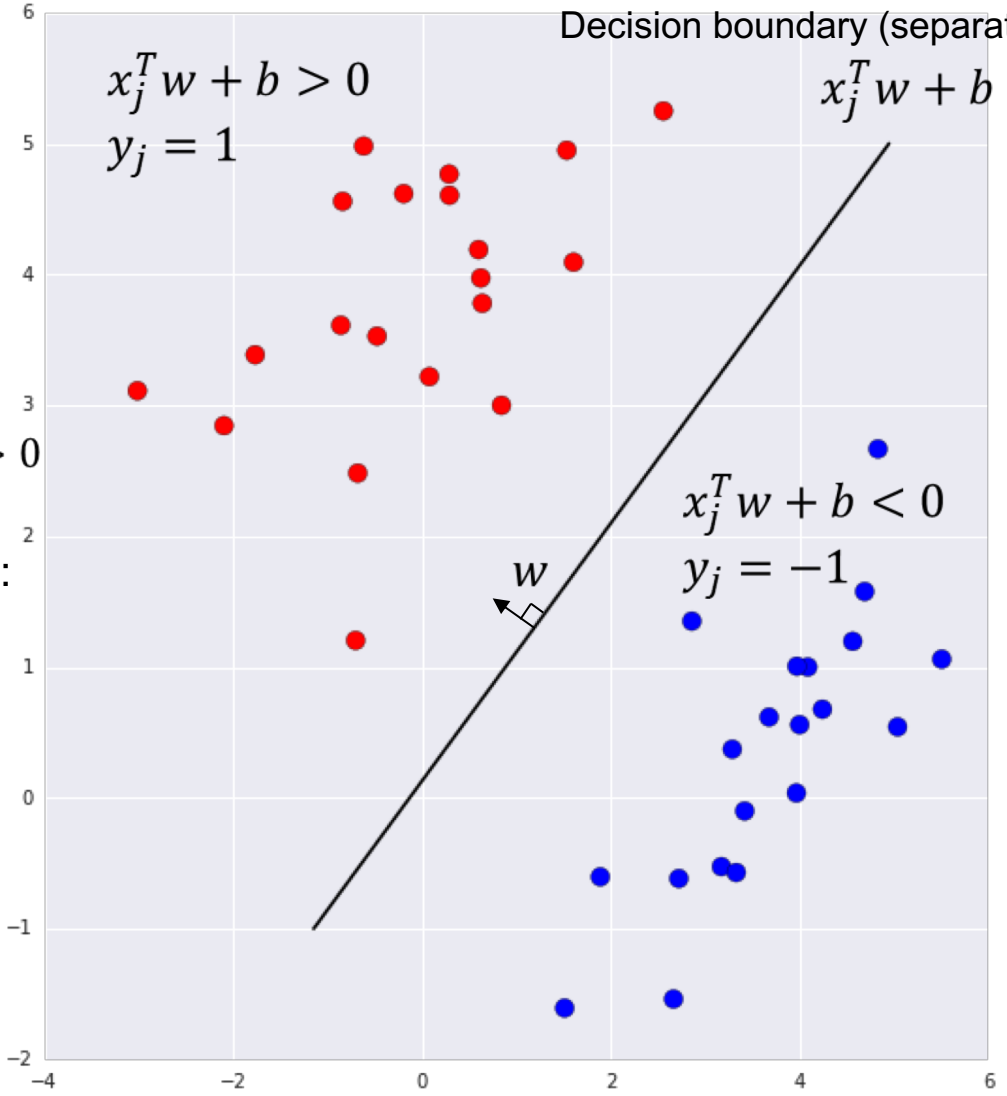
$$M = \min_j y_j(x_j^T w + b) > 0$$

Then for $y_j = 1$, we have:

$$x_j^T w + b \geq M$$

For $y_j = -1$, we have:

$$x_j^T w + b \leq -M$$



Represent each point as (x_j, y_j), where y_j, the class value we are trying to predict, is +1 or -1. Note that x_j is a vector of length 2 in this example.

How to maximize the margin?

To separate, for all points j, we must have:

$$y_j(x_j^T w + b) > 0$$

For the margin, define:

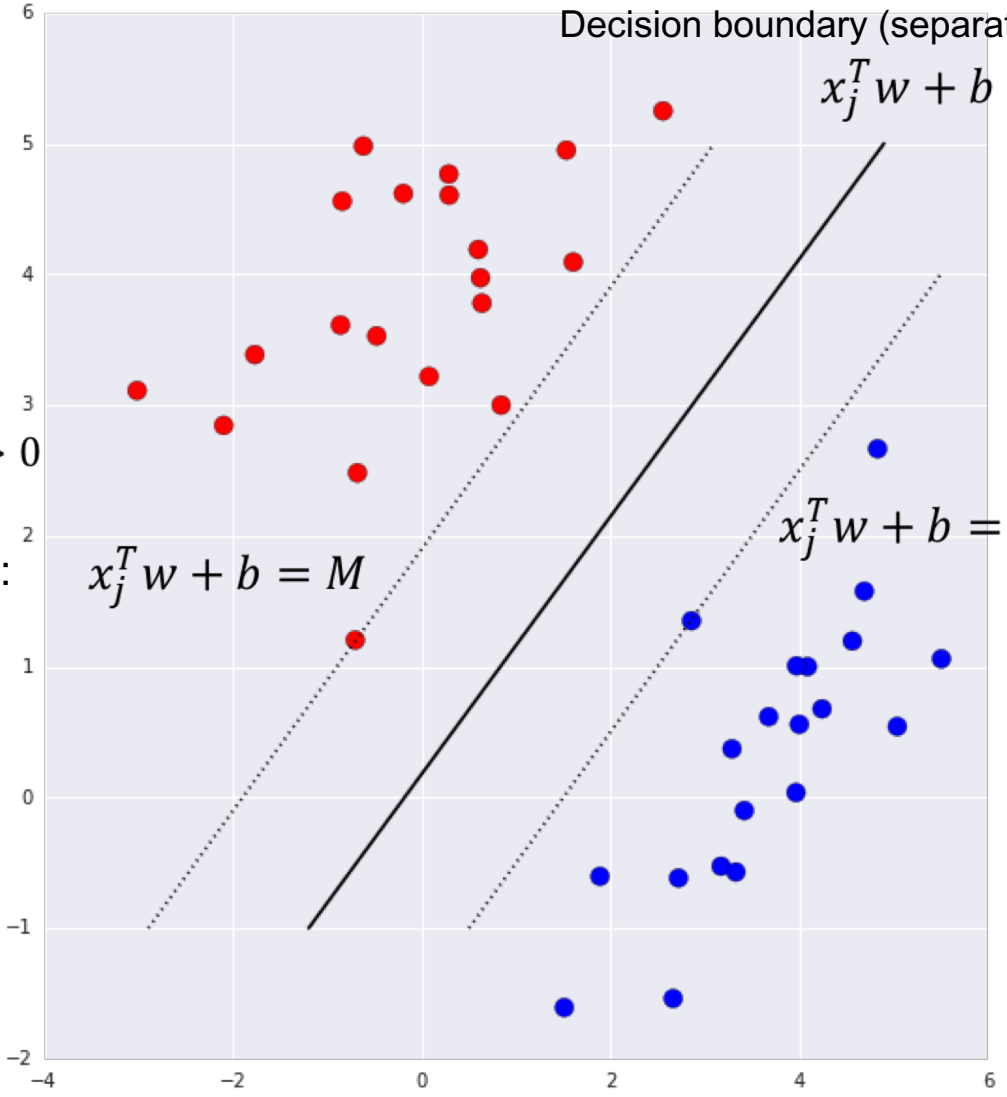
$$M = \min_j y_j(x_j^T w + b) > 0$$

Then for $y_j = 1$, we have:

$$x_j^T w + b \geq M$$

For $y_j = -1$, we have:

$$x_j^T w + b \leq -M$$



Represent each point as (x_j, y_j), where y_j, the class value we are trying to predict, is +1 or -1. Note that x_j is a vector of length 2 in this example.

How to maximize the margin?

Margin = 2M / ||w||.

This follows from computing distance between parallel lines.

Goal: maximize 2M / ||w|| subject to constraints, for all j:

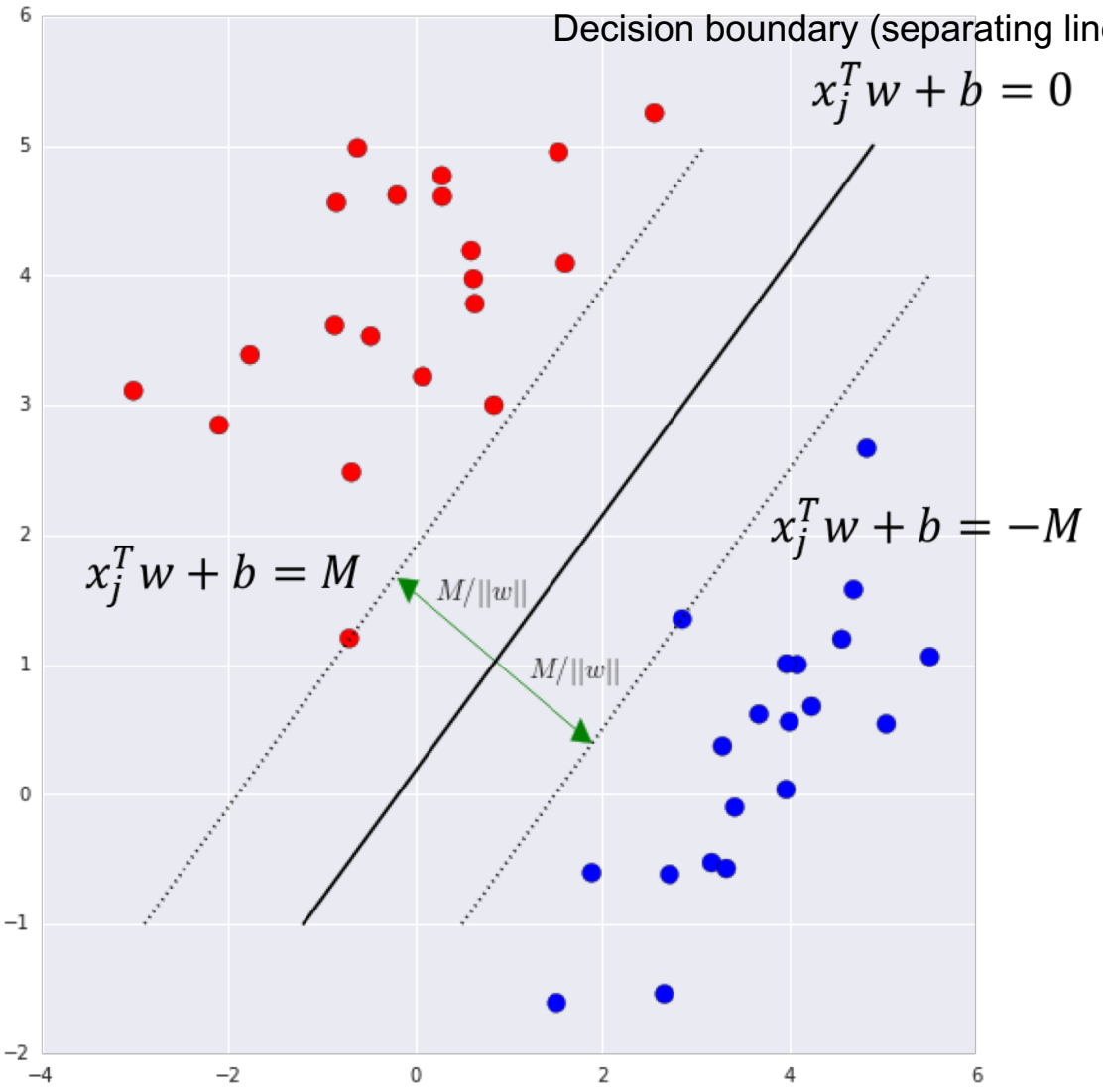
$$y_j(x_j^T w + b) \geq M$$

Simplify by change of variables, dividing w and b through by M.

New goal: minimize ||w|| subject to constraints, for all j:

$$y_j(x_j^T w + b) \geq 1$$

New margin: 2 / ||w||



How to maximize the margin?

Margin = 2M / ||w||.

This follows from computing distance between parallel lines.

Goal: maximize 2M / ||w|| subject to constraints, for all j:

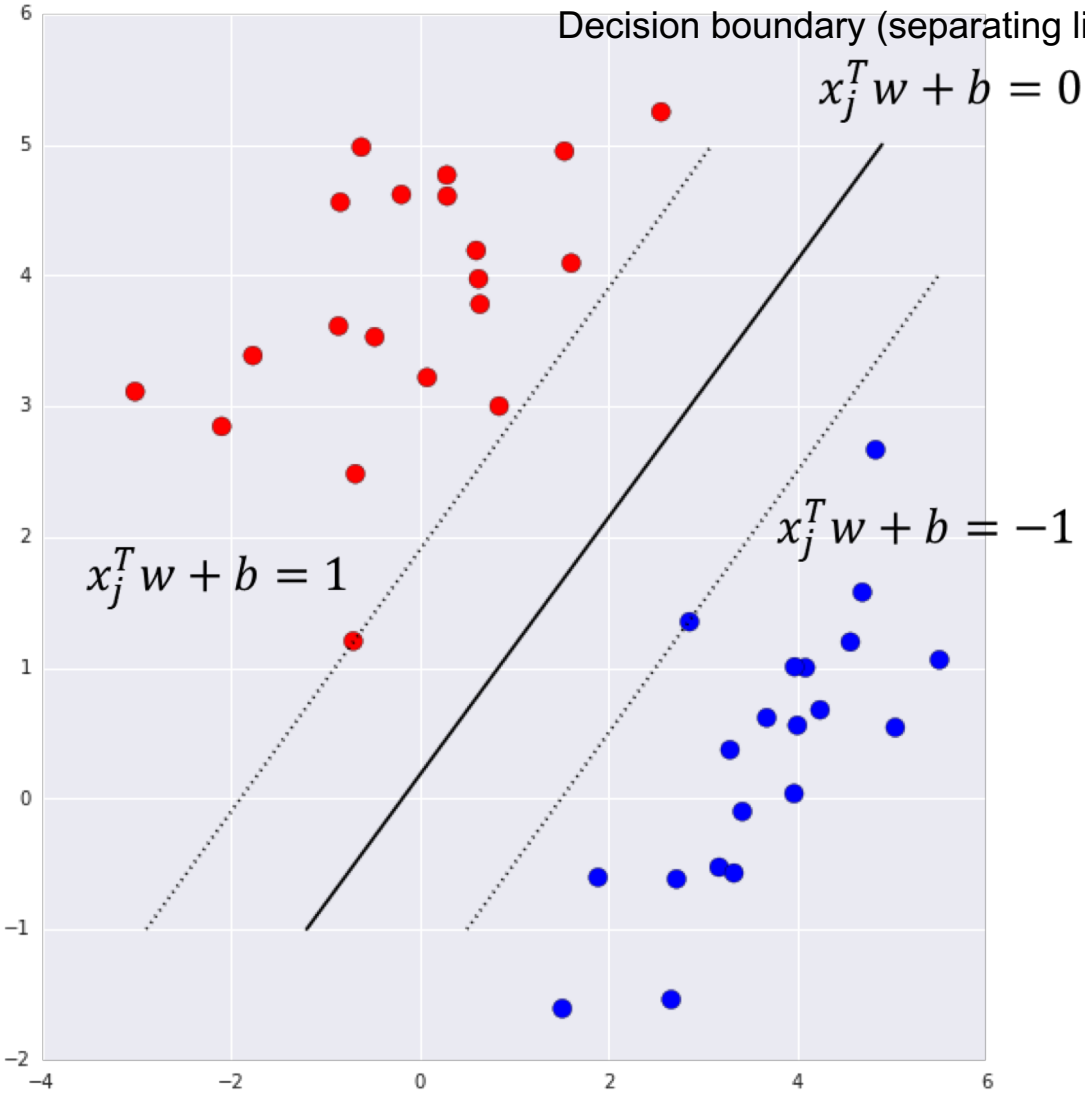
$$y_j(x_j^T w + b) \geq M$$

Simplify by change of variables, dividing w and b through by M.

New goal: minimize ||w|| subject to constraints, for all j:

$$y_j(x_j^T w + b) \geq 1$$

New margin: 2 / ||w||



How to maximize the margin?

Margin = 2M / ||w||.

This follows from computing distance between parallel lines.

Goal: maximize 2M / ||w|| subject to constraints, for all j:

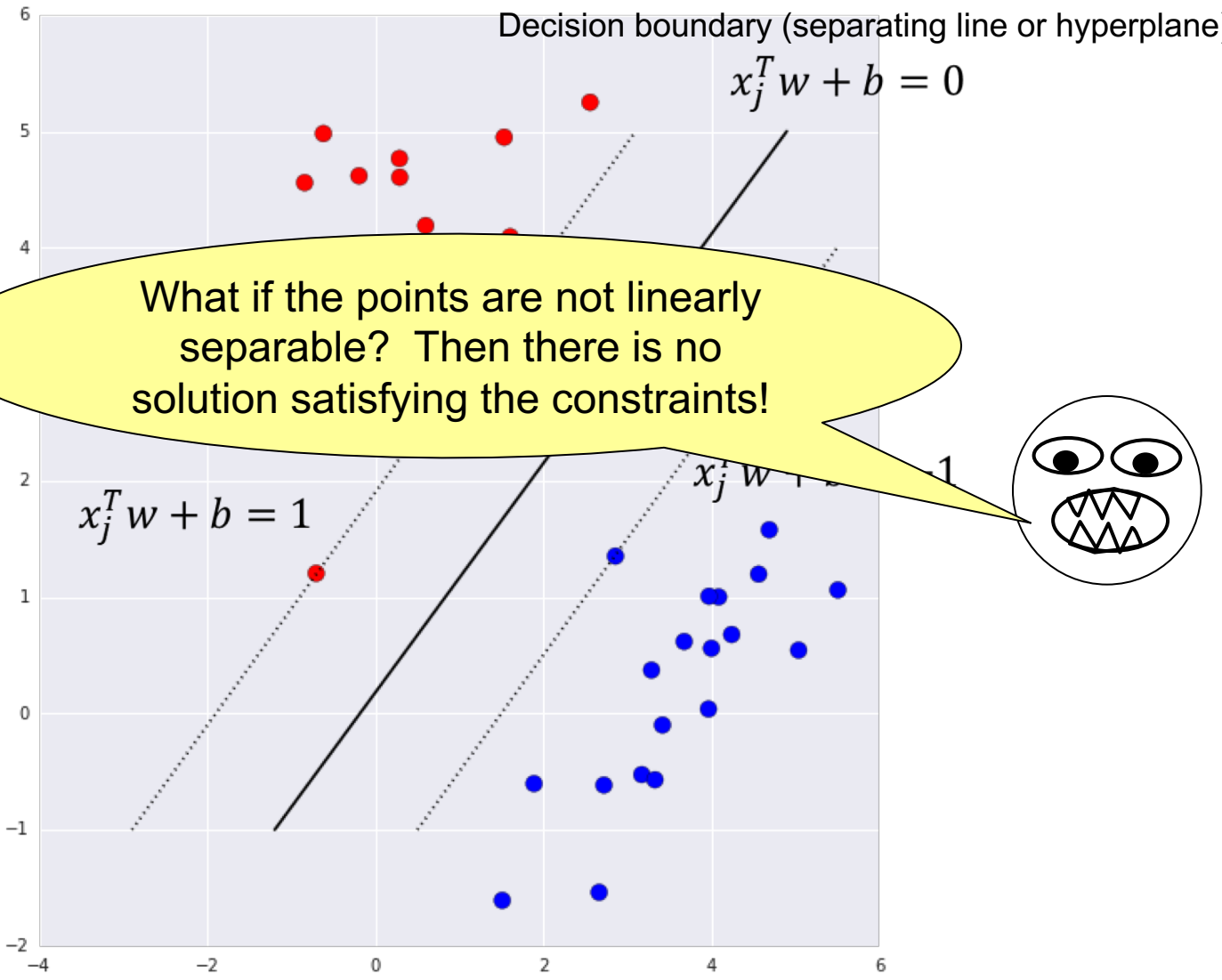
$$y_j(x_j^T w + b) \geq M$$

Simplify by change of variables, dividing w and b through by M.

New goal: minimize ||w|| subject to constraints, for all j:

$$y_j(x_j^T w + b) \geq 1$$

New margin: 2 / ||w||



Non-separable case: soft margins

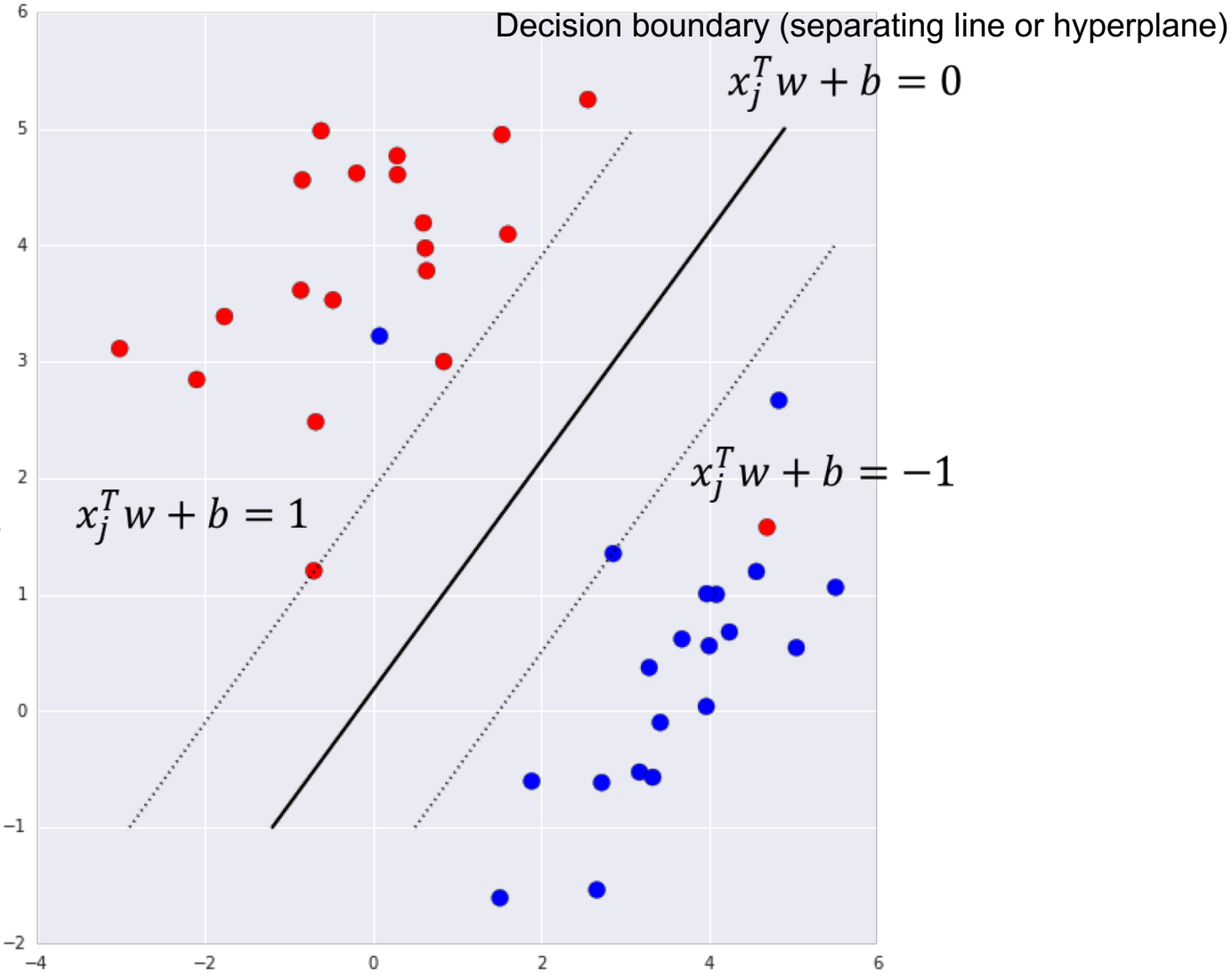
Goal (hard margin): minimize ||w|| subject to constraints, for all j:

$$y_j\left(x_j^T w + b\right) \geq 1$$

Goal (soft margin): minimize subject to constraints, for all j:

$$y_j\left(x_j^T w + b\right) \geq 1 - \xi_j$$

$$\xi_j \geq 0$$



Non-separable case: soft margins

Goal (hard margin): minimize ||w|| subject to constraints, for all j:

$$y_j\left(x_j^T w + b\right) \geq 1$$

Goal (soft margin): minimize subject to constraints, for all j:

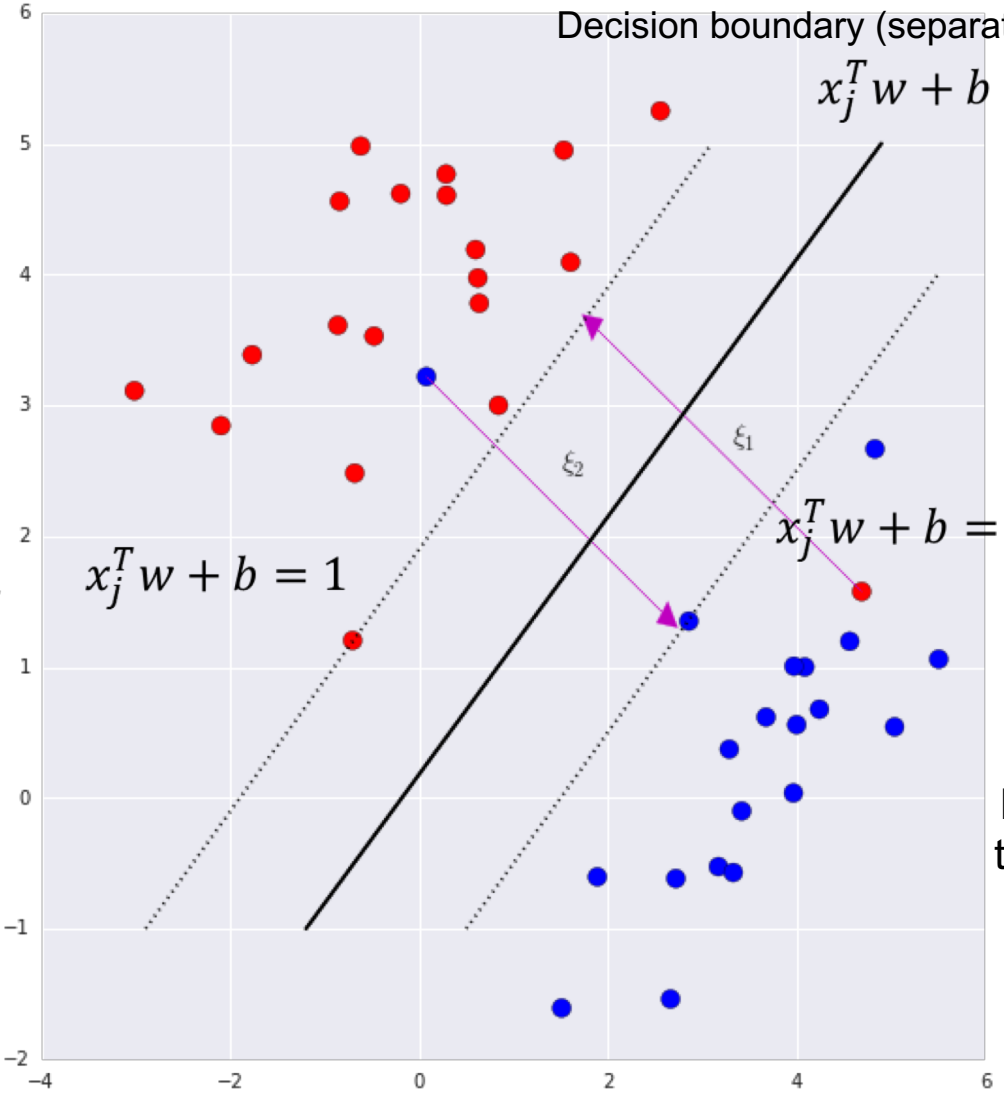
$$y_j\left(x_j^T w + b\right) \geq 1 - \xi_j$$

$$\xi_j \geq 0$$

But what should we minimize? ||w||?

Answer: minimize

$$\frac{1}{2}\|w\|^2 + C\sum_j \xi_j$$



This is a **quadratic programming** (QP) problem, optimizing a quadratic function with linear constraints.

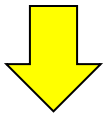
We can use off-the-shelf QP solvers, or faster methods for large problems, to find the optimal w, b, and ξ.

Classify test points by $sign(x_j^T w + b)$.

Soft margins in practice

Goal (hard margin): minimize ||w|| subject to constraints, for all j:

$$y_j\left(x_j^T w + b\right) \geq 1$$



Goal (soft margin): minimize subject to constraints, for all j:

$$y_j\left(x_j^T w + b\right) \geq 1 - \xi_j$$

$$\xi_j \geq 0$$

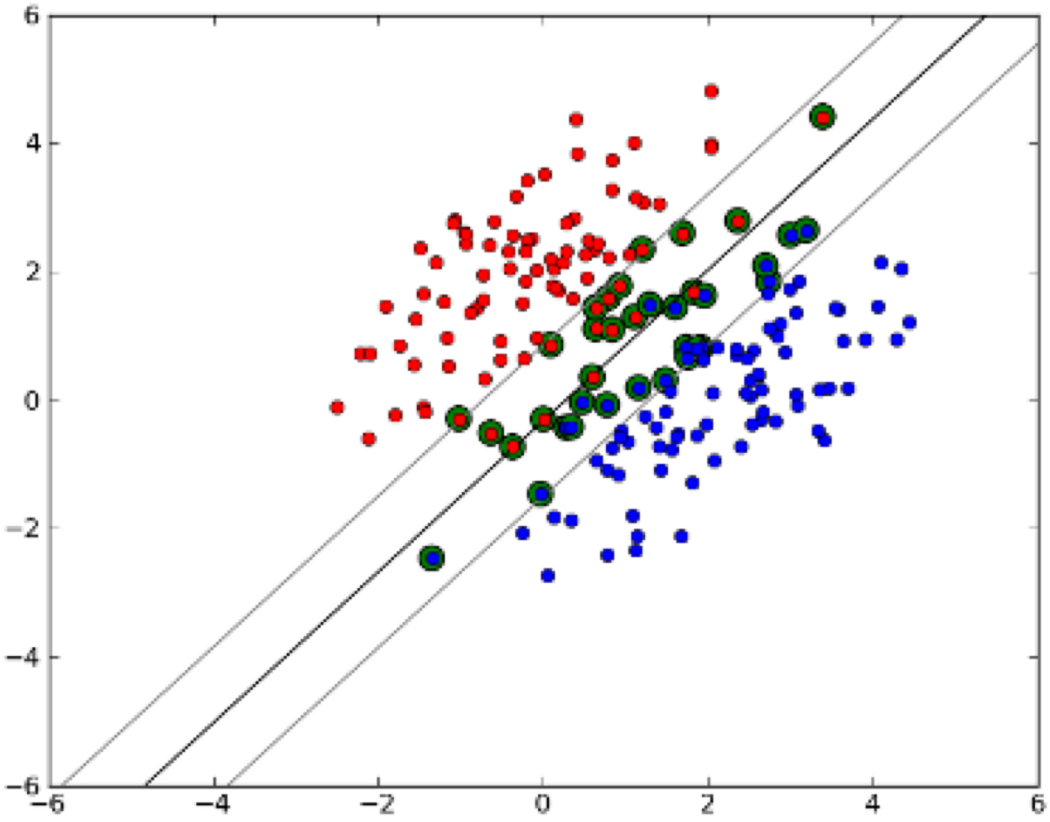
But what should we minimize? ||w||?

Answer: minimize

$$\frac{1}{2}\|w\|^2 + C\sum_j \xi_j$$

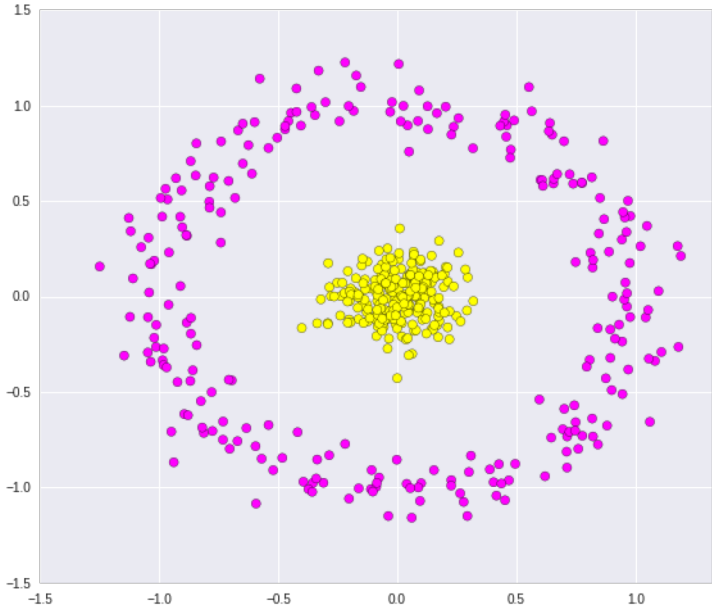
In practice, there may be many training points with $\xi_j > 0$ (all of these are support vectors).

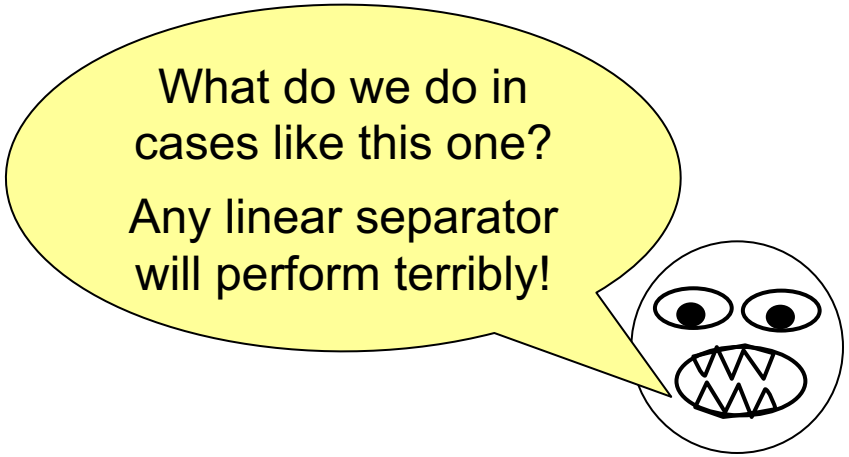
Training points with $\xi_j > 1$ are misclassifications.

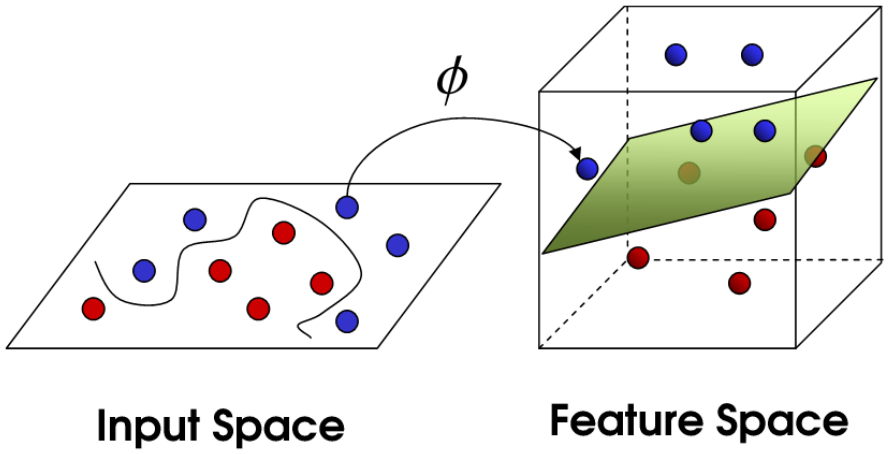


http://www.mblondel.org/journal/2010/09/19/support-vector-machines-in-python/

Non-linear decision boundaries



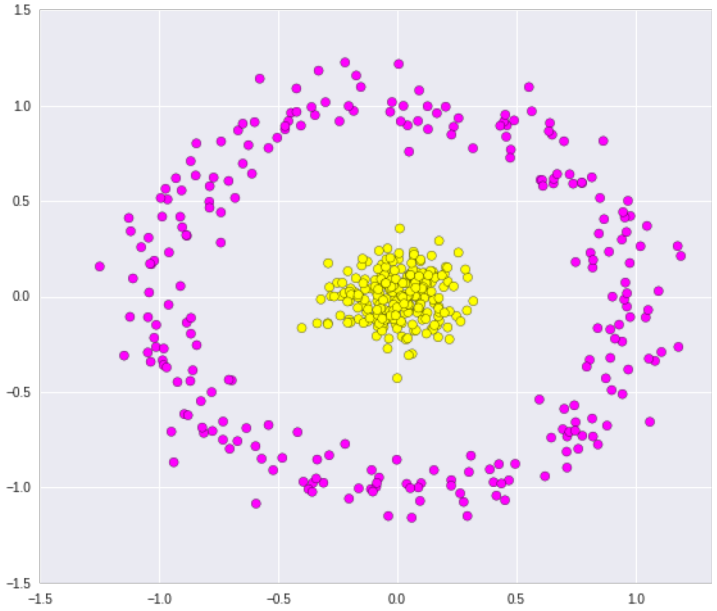




Solution:

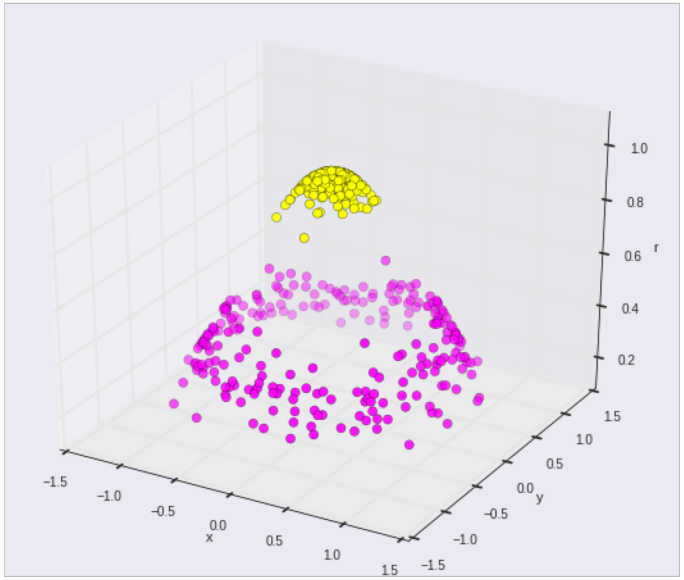
1) Map input space to a high-dimensional feature space.
2) Learn a linear decision boundary (hyperplane) in the high-dimensional space.
3) Map back to lower-dimensional space, giving a non-linear boundary.

Non-linear decision boundaries

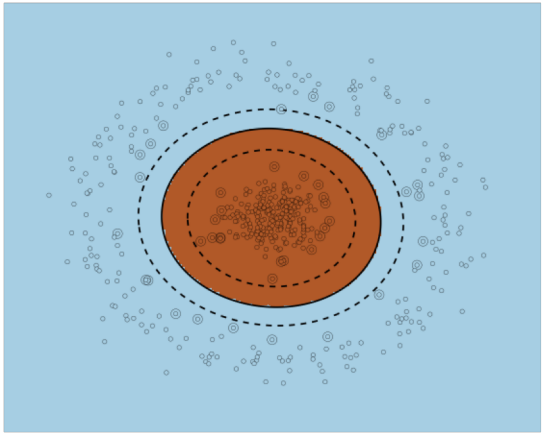


$$\phi : (x, y) \rightarrow (x, y, r)$$

$$r = e^{-(x^2+y^2)}$$



The resulting classifier perfectly separates the training data.



Non-linear decision boundaries

Non-linear QP problem: $\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C\sum_j \xi_j$ subject to: $y_j\left(w^T \boldsymbol{\Phi}(x_j) + b\right) \geq 1 - \xi_j$

$\xi_j \geq 0$

Problem: not efficiently computable, since $\boldsymbol{\Phi}(x_j)$ may be high- or infinite-dimensional!

Solution: transform to equivalent ("dual") QP problem:

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - \sum_j \alpha_j \quad \text{subject to: } 0 \leq \alpha_j \leq C \quad \text{where: } Q_{ij} = y_i y_j(\boldsymbol{\Phi}(x_i) \cdot \boldsymbol{\Phi}(x_j))$$

$$\sum_j \alpha_j y_j = 0 \qquad = y_i y_j K(x_i, x_j)$$

Very cool trick (the "kernel trick"): instead of mapping both x_i and x_j into a high-dimensional space and computing the dot product in that space, we can just compute a function $K(x_i, x_j)$ of the original data points.

This makes the QP efficiently solvable. To classify a test point x, we just need to compute $sign(\sum_j \alpha_j y_j K(x_j, x) + \rho)$.

Sum is just over the support vectors; other points have $\alpha_j = 0$.

Some common kernel functions

Linear kernel: $\phi : x \to x \qquad K(x_i, x_j) = x_i \cdot x_j$

Non-linear kernels

Polynomial kernel: $K(x_i, x_j) = (\gamma(x_i \cdot x_j) + r)^d$

Sigmoid kernel: $K(x_i, x_j) = \tanh(\gamma(x_i \cdot x_j) + r)$

Gaussian kernel: $K(x_i, x_j) = \exp\left(-\gamma \|x_i - x_j\|^2\right)$

The Gaussian kernel is usually called the "radial basis function", or **RBF**, kernel. It is one of the most widely used choices of kernel and a good default option.

Very cool trick (the "kernel trick"): instead of mapping both x_i and x_j into a high-dimensional space and computing the dot product in that space, we can just compute a function $K(x_i, x_j)$ of the original data points.

This makes the QP efficiently solvable. To classify a test point x, we just need to compute $sign(\sum_j \alpha_j y_j K(x_j, x) + \rho)$.

Sum is just over the support vectors; other points have $\alpha_j = 0$.

Variants and extensions of SVMs

SVMs are mainly used for **non-probabilistic, binary classification**.

To do multi-class classification:

For each class k, learn a binary classifier (class k vs. rest).

To predict the output for a new test example x, predict with each SVM.

Choose whichever one puts the prediction the furthest into the positive region.

To estimate class probabilities:

SVMs are not really the best for this, but can do logistic regression using outputs of k(k-1) pairwise SVMs.

Lots of models + additional cross-validation needed → this approach is very computationally expensive. (See Wu et al., 2004, for details.)

Support vector machines can also be used for **regression** (Smola and Schölkopf, 2003) and for **anomaly detection** (the "one-class SVM", Schölkopf et al., 2001).

Both are implemented in scikit-learn, but are beyond the scope of this class.

Some advantages of SVMs

- Very good performance: though lately outshined by convolutional neural networks on some benchmarks (e.g., the MNIST digit recognition dataset) they often beat basically everything else.
- Theoretical guarantees about their generalization performance (accuracy for labeling test data) based on statistical learning theory.
- SVMs rely on convex optimization and do not get stuck in suboptimal local minima (neural networks have a big problem with these; similarly, decision trees rely on greedy search).
- Fairly robust to the curse of dimensionality → can effectively solve prediction problems with a large number of features.
- Flexible: can choose kernel to fit very complex decision boundaries.
- Will generally avoid overfitting with well-chosen parameters (but can certainly overfit for poorly chosen values, e.g., if C is too large).
- Classification of test points relies only on the support vectors → fast and memory efficient, especially when # of support vectors is small.

Some disadvantages of SVMs

- Training the model is **computationally expensive** – dependent on # of support vectors, but typically quadratic to cubic in the number of data points.
- Sensitive to choice of **parameters**, particularly the constant C and kernel bandwidth (γ for RBF kernel in sklearn).
    - C trades off misclassification rate against simplicity of the decision surface. Low C → smooth decision surface; High C → more training examples classified correctly.
    - Larger γ = lower bandwidth (increased weight on nearest training examples).
    - Proper choice of C and γ is critical to the SVM's performance.
    - For sklearn, use GridSearchCV with C and γ spaced exponentially far apart.
- Not much **interpretability** for non-linear SVM: can enumerate the support vectors or (in low dimensions) visualize the decision boundary, but actually obtaining these involves calling a black-box optimization routine.

References

- Scikit-learn documentation: http://scikit-learn.org/stable/modules/svm.html
- C.J.C. Burges. A tutorial on support vector machines for pattern recognition. *Data Mining & Knowledge Discovery*, 2: 955-974, 1998. http://research.microsoft.com/en-us/um/people/cburges/papers/svmtutorial.pdf
- A.W. Moore. Support Vector Machines (tutorial slides). https://www.autonlab.org/tutorials/svm.html
- V. Vapnik. *Statistical Learning Theory*. Wiley: 1998.
- T.-F. Wu, C.-J. Lin, and R.C. Weng. Probability estimates for multi-class classification by pairwise coupling. *Journal of Machine Learning Research* 5: 975-1005, 2004.
- A.J. Smola and B. Schölkopf. A tutorial on support vector regression, *Statistics and Computing*, 2003. http://alex.smola.org/papers/2003/SmoSch03b.pdf
- B. Schölkopf et al. Estimating the support of a high-dimensional distribution. *Neural Computation* 13: 1443-1471, 2001.

Up next: a short break, and then Python examples for support vector machines.