Support Vector Machines

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Lecture 12

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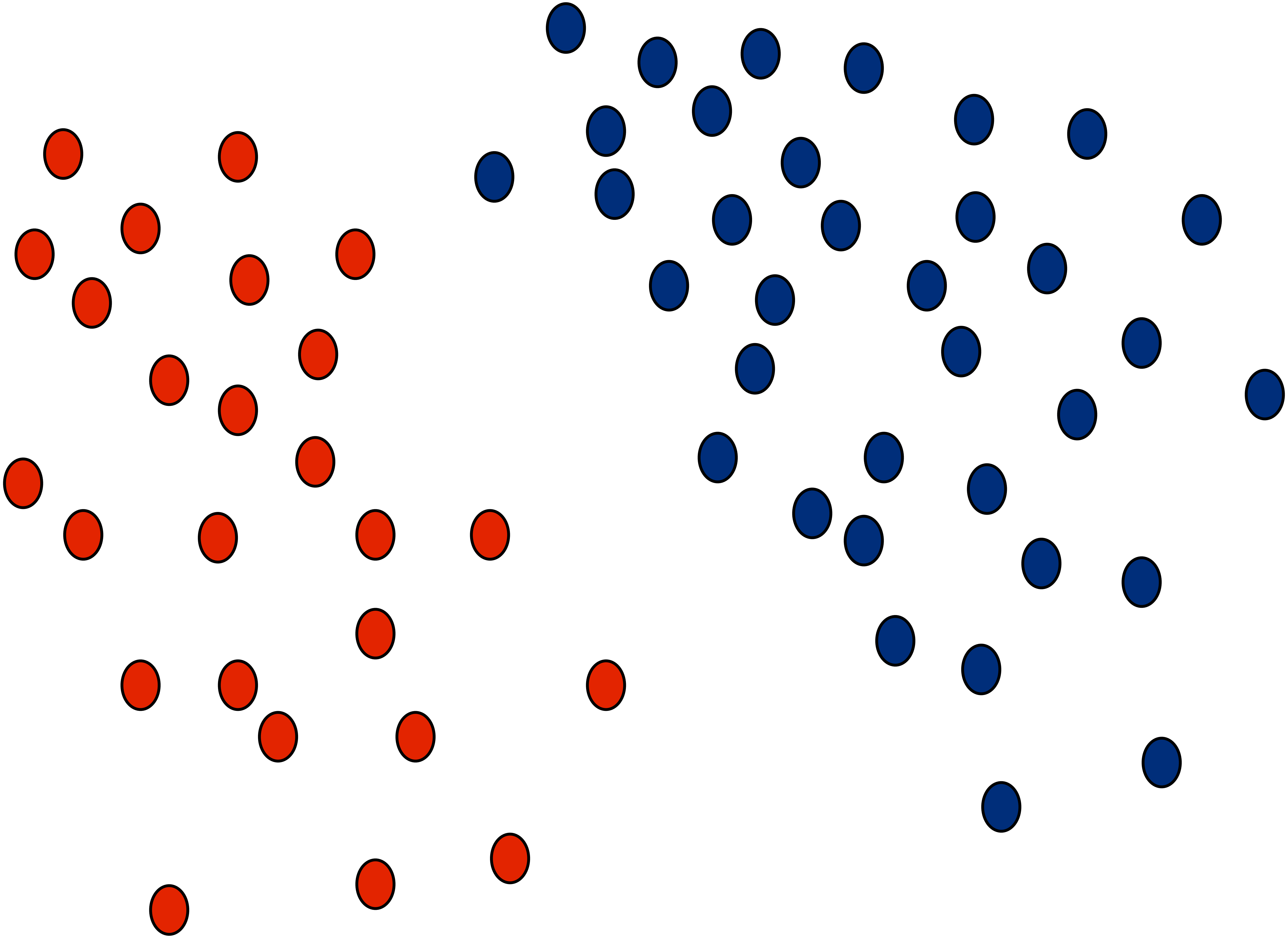
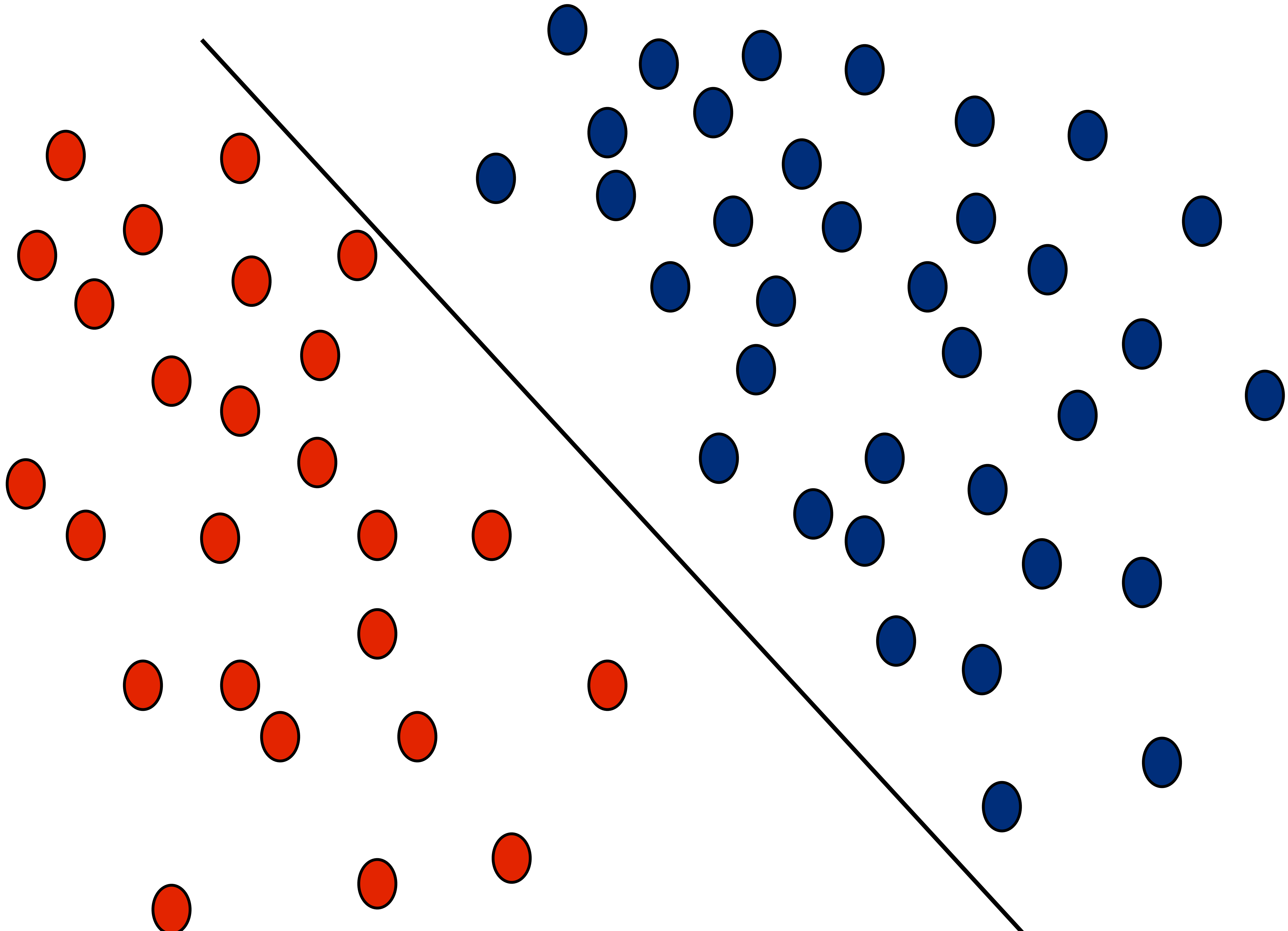
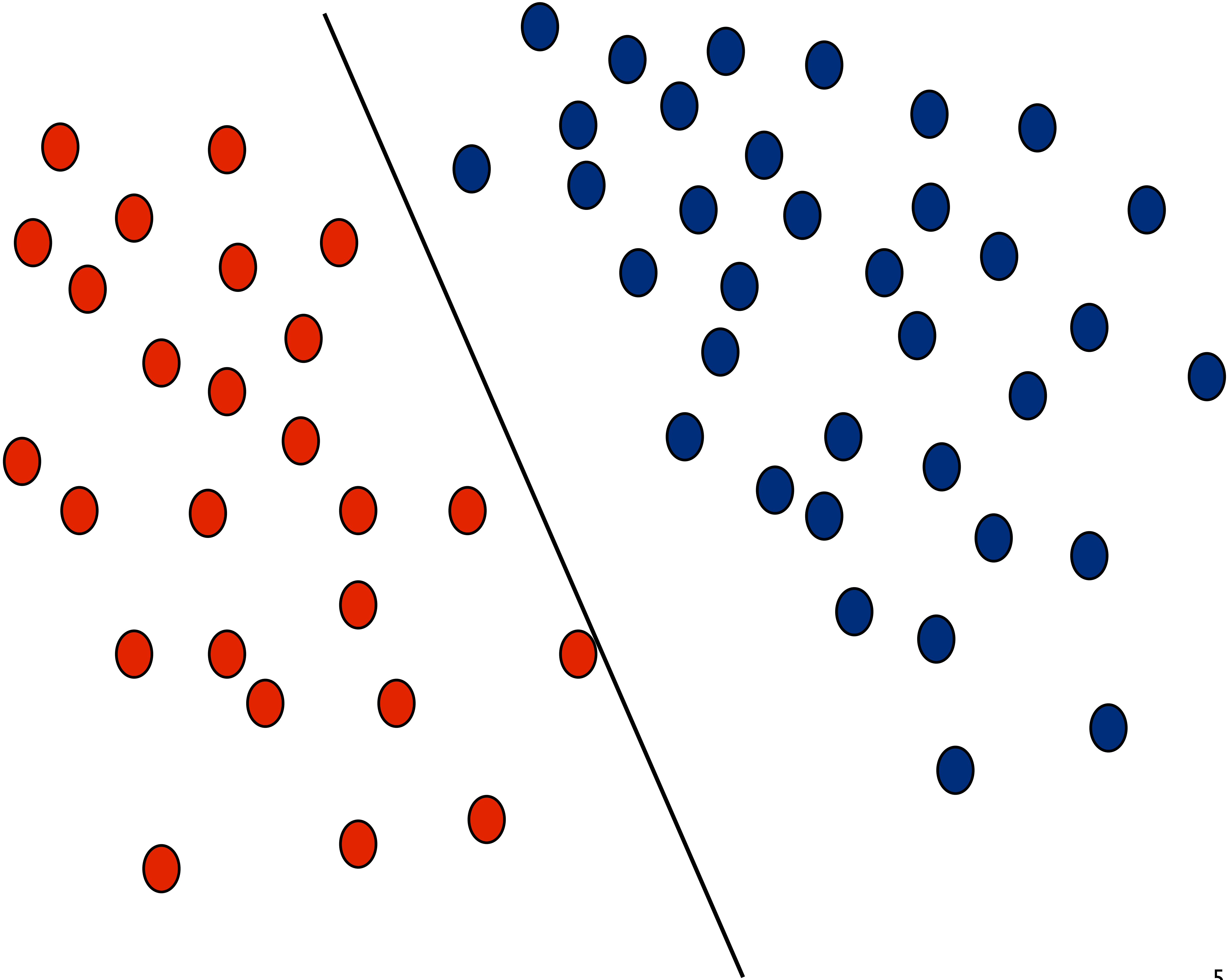
Linear Separability

- Consider binary classification of two dimensional feature vectors
  - e.g. features = {good, bad}
  - classes = {positiveSentiment, negativeSentiment}
- If we can find a straight line that can separate all positive instances (reviews) from all negative instances (reviews) then we call such a dataset to be *linearly separable*







Higher Dimensions

- Reviews contain more than two features (words)
- In N-dimensional space, we must find (n-1) dimensional hyperplane that separates the two classes (if they are linearly separable)
- n=2 (two dimensional feature space), we had straight lines (n=1 dimensional hyperplanes)
- Hyperplane that separates the two classes might not be unique (as we saw in our previous example)

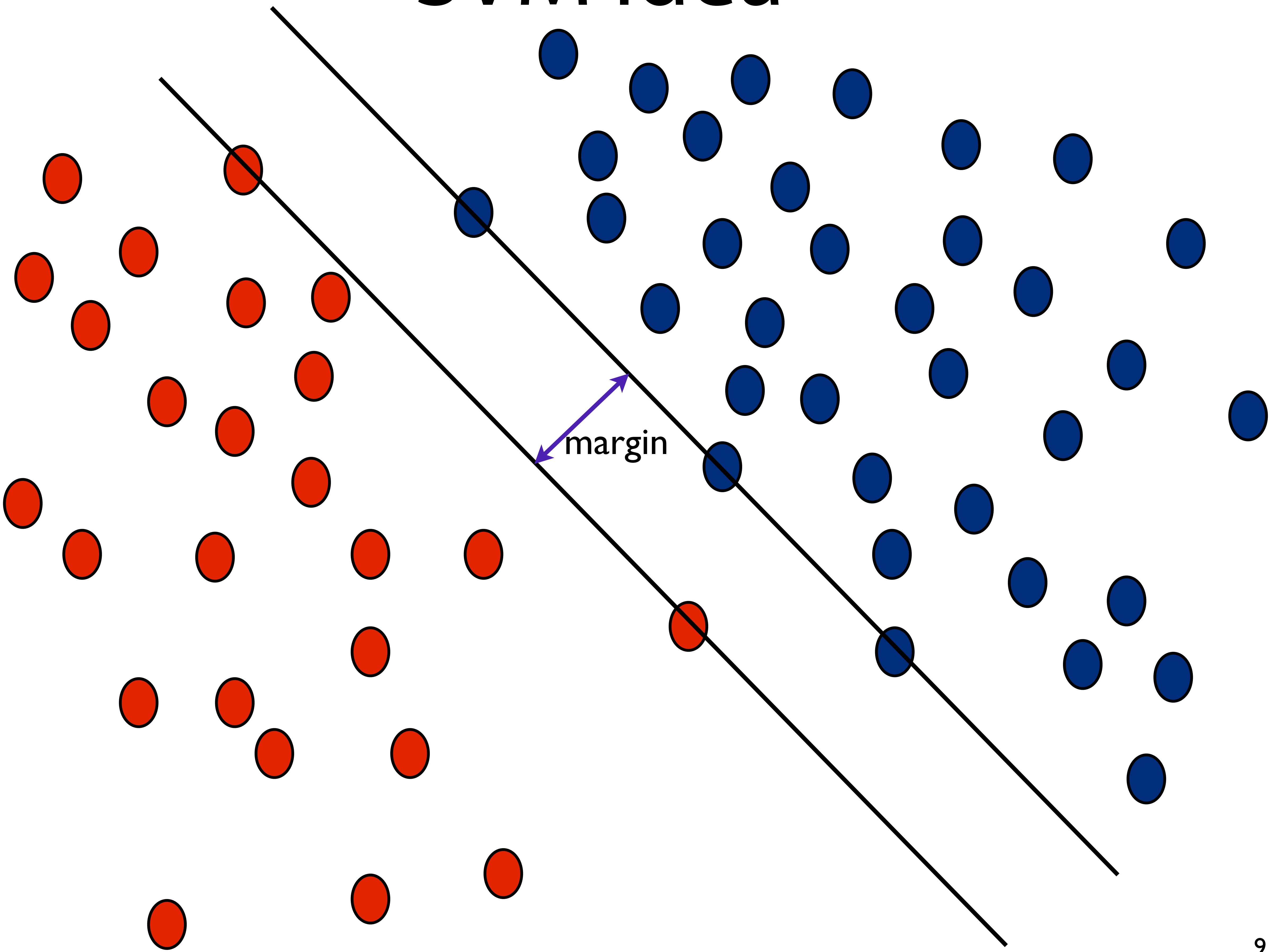
Large Margin Classifiers

- Find two hyperplanes that separates the positive class and the negative class
- Try to maximise the minimum separation (distance) between the two hyperplanes
  - The distance between the hyperplanes is called the margin
- Maximising the margin minimises the risk of misclassifying an instance at test time
  - reduces overfitting

Support Vector Machines

- Support Vector Machines (SVMs) are one of the many large margin classification methods
- Uses a constrained convex optimisation method
- Can handle non-linear separable datasets using
  - slack variables
  - kernel functions

SVM Idea

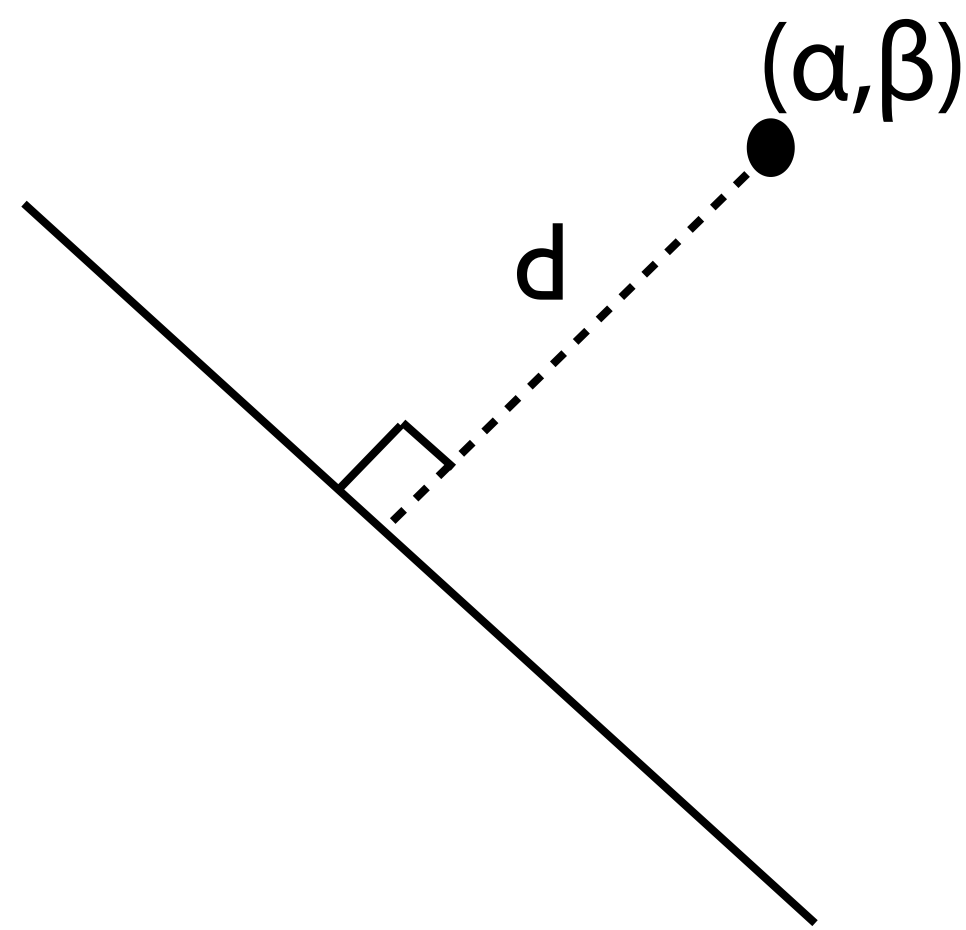


Distance to a straight line

- Given a straight line *l* ax+by+c=0 show the perpendicular distance *d* to *l* from a point (α,β) is

Home Work 1

$$d = \frac{a\alpha + b\beta + c}{\sqrt{a^2 + b^2}}$$



Distance to a hyperplane

- A hyperplane can be expressed as the inner-product between a weight vector (coefficients) and a feature vector (variables corresponding to the dimensions)
  - $\mathbf{w}^\top \mathbf{x} = 0$
- Then the distance to this hyperplane from a point *p*, given by the vector **p** can be computed as

$$\frac{\boldsymbol{w}^\top \boldsymbol{p}}{||\boldsymbol{w}||}$$

  - where $||\mathbf{w}||$ is the norm (L2 length) of the vector **w**
- Observe that this formula reduces to the one we derived in the two-dimensional case in the previous slide

SVM background

- Let us assume we are given a training dataset (t_n, x_n) of n=1,...,N instances
  - target labels $t_n = \{-1, +1\}$ for binary classification
- The feature vector for the instance x is represented by $\phi(x)$
- Our classification decision of x is made according to the score y(x) given by
  - $y(x) = \mathbf{w}^T\phi(x) + b$
- Here, **w** is the weight vector and b is the bias (scalar) term that adjust any fixed bias from the 0 threshold
  - If y(x) > 0 then we classify x to be positive and
  - otherwise negative

SVM Derivation

- If a point (instance) is correctly classified by the hyperplane then
  - $t_n y(x_n) > 0$
- The distance from a correctly classified point to the hyperplane is given by

$$\frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}.$$

SVM Derivation

- We need to find the weight vector **w** and bias term b such that this margin is maximised for all the training instances in our train dataset

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b \right) \right] \right\}$$

This is a difficult optimisation problem involving min-max. Moreover, it is scale-invariant meaning that by setting w→kw and b→kb the term inside min does not change!

Simplification!

- Scale the parameters such that a point on the decision hyperplane satisfies

$$t_n \left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b\right) = 1$$

- All correctly classified data points will then satisfy

$$t_n \left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b\right) \geqslant 1, \qquad n = 1, \ldots, N.$$

- This is called the *canonical representation* of the decision hyperplane

SVM Derivation 3

- Now the margin becomes

$$\frac{t_n y(x_n)}{||\boldsymbol{w}||} = \frac{t_n(\boldsymbol{w}^\top \phi(x_n) + b)}{||\boldsymbol{w}||} = \frac{1}{||\boldsymbol{w}||}$$

- Great!
- Now our final objective becomes to find **w** and b such that we maximise the margin subjected to the set of constraints that ensures our train data instances are correctly classified
- Maximising margin = minimising the norm ||**w**||

SVM Optimisation Problem

- Find **w** and b such that
  - minimise

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

  - subjected to

$$t_n \left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) + b \right) \geqslant 1, \qquad n = 1, \ldots, N.$$

Constrained Optimisation

- Find x that minimises f(x)
  - unconstrained optimisation
- Find x that minimises f(x) subjected to g(x) = 0
  - constrained optimisation

unconstrained vs. constrained

- minimise $f(x,y) = x^2 + y^2$
- such that $g(x,y) = y - x - 1 = 0$

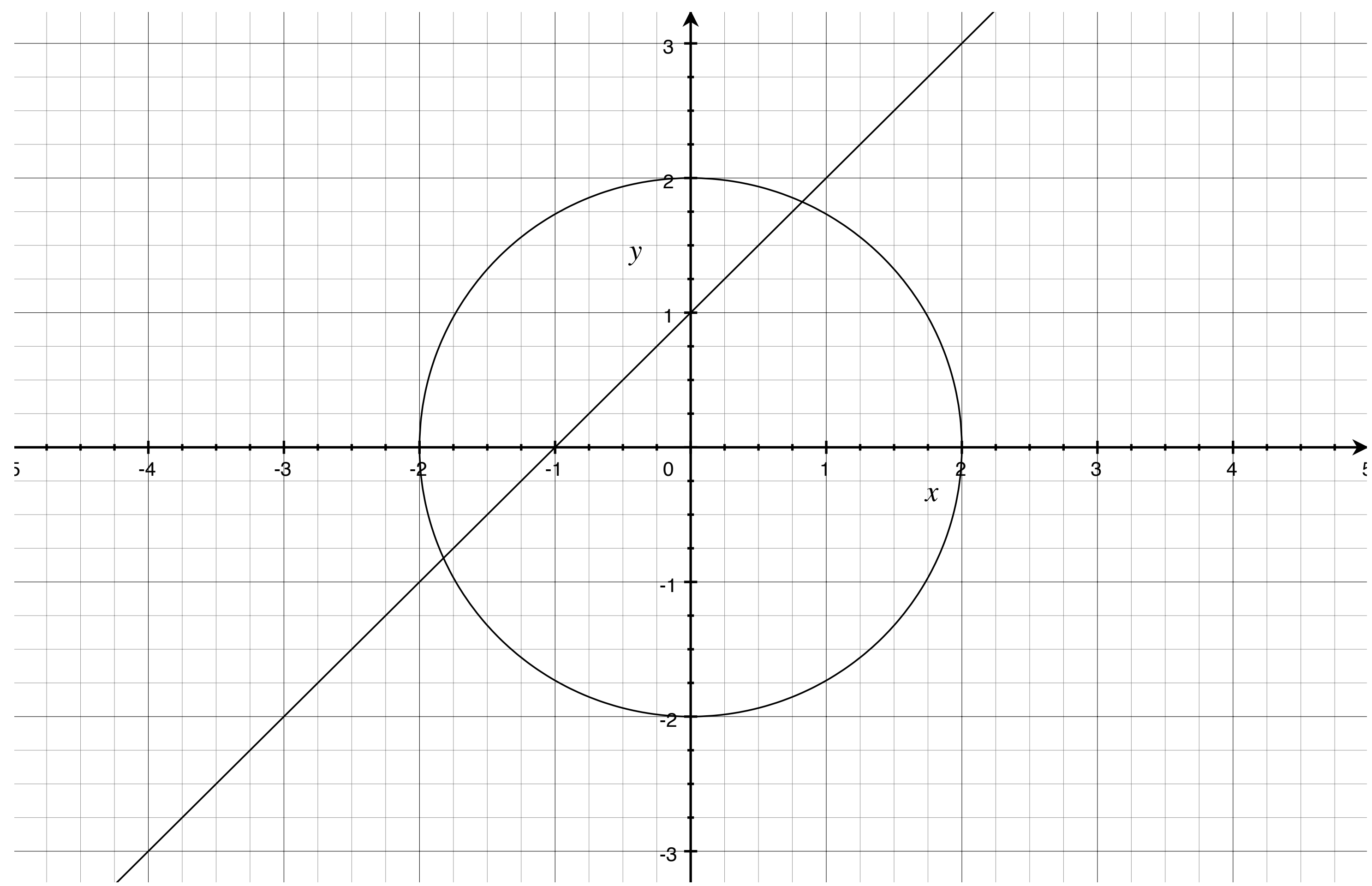
$$f(x,y) = x^2 + (x+1)^2 = 2x^2 + 2x + 1$$

$$\frac{\partial f}{\partial x} = 4x + 2 = 0$$

$$x = -1/2$$

$$y = x + 1 = 1/2$$

$$\min f(x,y) = (-0.5)^2 + (0.5)^2 = 0.5$$



Lagrange Multipliers

- Problem:
  - Minimise f(x) subjected to g(x) ≧ 0
- Lagrangian function for the problem becomes
  - $L(x, \lambda) = f(x) - \lambda g(x)$
  - $\lambda \geq 0$ is called the Lagrange variable
- Procedure
  - Compute x and λ by solving

$$\frac{\partial L(x,\lambda)}{\partial \lambda} = 0$$

$$\frac{\partial L(x,\lambda)}{\partial w} = 0$$

Idea

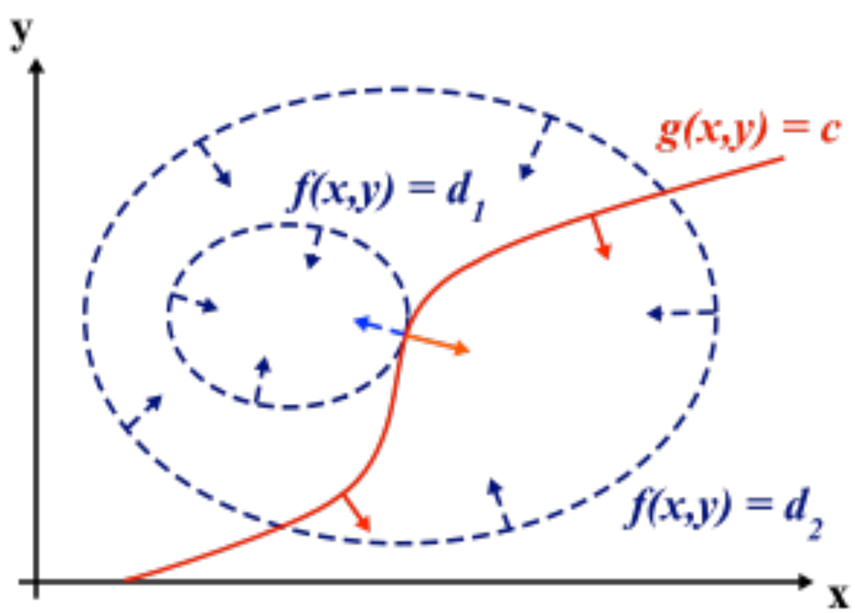


figure from Wikipedia

Minimising a two variable function f(x,y) w.r.t. x and y means that we are drawing the contours for f(x,y).

Minimising while satisfying g(x,y) = c happens when the two curves touch each other.

At this point the two gradients must be parallel and in opposite directions

Home Work

- Use Lagrangian multiplier method to solve the optimisation problem in slide 19

Back to SVM Derivation

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{ t_n(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) + b) - 1 \right\}$$

$$\frac{\partial L(\boldsymbol{w}, b, \boldsymbol{a})}{\partial \boldsymbol{w}} = 0 \Rightarrow \mathbf{w} = \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)$$

$$\frac{\partial L(\boldsymbol{w}, b, \boldsymbol{a})}{\partial b} = 0 \Rightarrow 0 = \sum_{n=1}^{N} a_n t_n.$$

SVM

- Plugging these back to the Lagrangian function we get

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

- Which must be solved subjected to constrains

$$\begin{aligned} a_n &\geqslant 0, \qquad n = 1, \ldots, N, \\ \sum_{n=1}^{N} a_n t_n &= 0. \end{aligned}$$

Observations

- We must find Lagrange multipliers a_n (collectively denoted by the vector $\mathbf{a}$) such that $L(\mathbf{a})$ is minimised.
- We have the inner-product between two instances x_n and x_m appearing in the objective function
  - $k(x_n, x_m) = \phi(x_n)^T \phi(x_m)$
  - Only the inner products matter. We do not need the explicit form of feature vectors $\phi(x)$
  - Can be *kernalised* using numerous kernel functions to overcome the non-linear separability issue.

Observations

- Note that if the Lagrange multiplier $a_n = 0$, then the n-th instance has no effect on the objective function L
- The instances that correspond to non-zero Lagrange multipliers are the ones that we need to store in our final model
  - Support Vectors
    - The instances that appear on top of the decision hyperplanes and determine its shape

Classification with SVMs

- During test time, to classify a test instance x, we simply compute the inner-product between x and each of the support vectors x_n

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b.$$

We still do not need the explicit representation of x or x_n and can work with the values returned by the kernel function

Home Work

- Using the decision function $y(x) = \mathbf{w}^T\phi(x) + b$ and the result we obtained for **w** in slide 23, derive the classification function for SVMs in the kernel form as shown in slide 27.

Kernel Functions

- Linear Kernel

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = {\boldsymbol{x}_n}^\top \boldsymbol{x}_m$$

  - Does not use any transformations

- Polynomial Kernel

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = ({\boldsymbol{x}_n}^\top \boldsymbol{x}_m + c)^d$$

  - Quadratic (d=2), and Cubic (q=3) are widely used.
  - Can account for the combinations of features such as bigrams in text mining tasks

- Sigmoid Kernel

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \tanh({\boldsymbol{x}_n}^\top \boldsymbol{x}_m + c)$$

- Exponential Radial Basis Function (RBF) Kernel

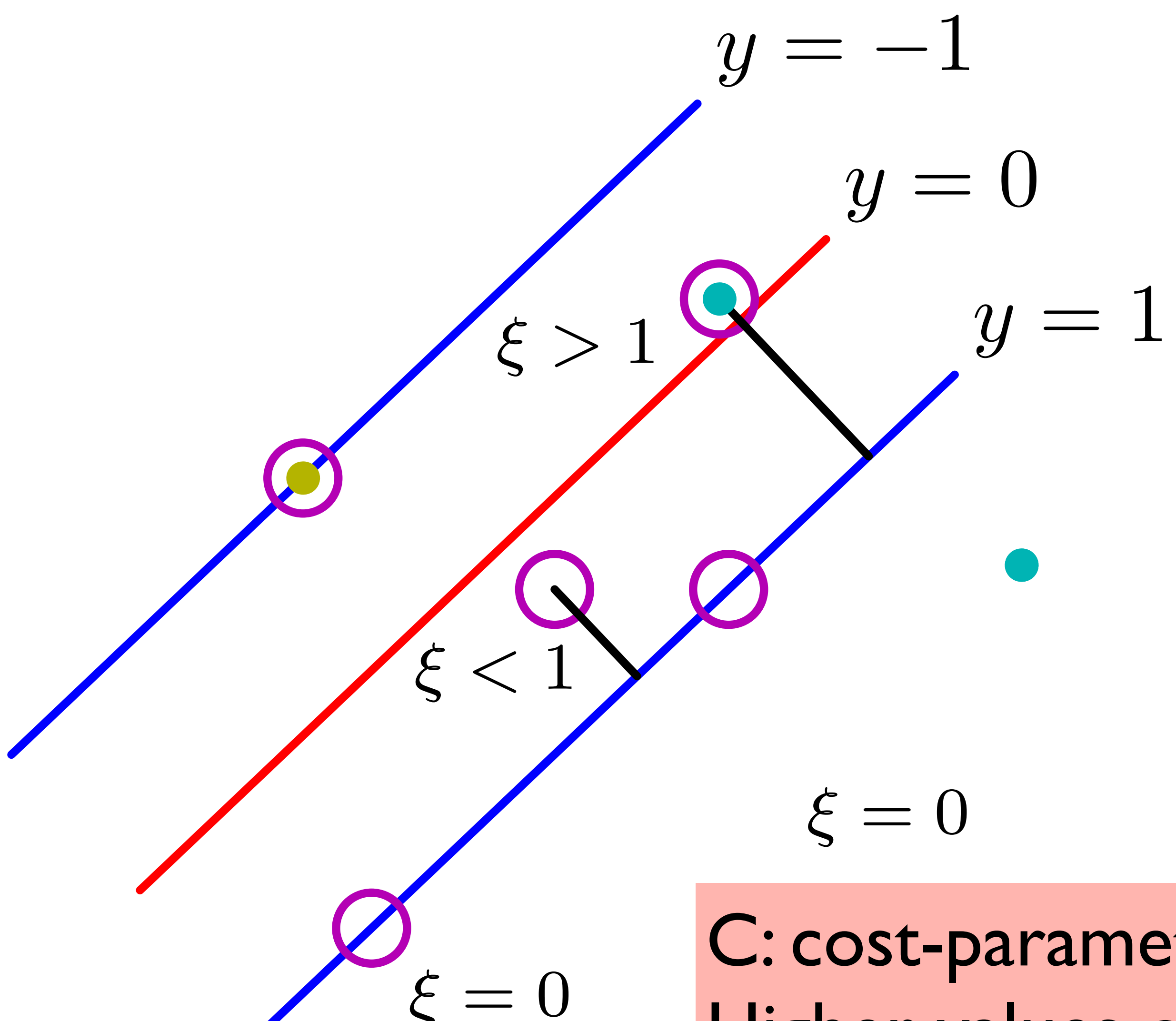
$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \exp\left(-\frac{||(\boldsymbol{x}_n - \boldsymbol{x}_m)||}{2\sigma^2}\right)$$

  - Subsumes all possible kernel functions

Slack variables

- Sometimes it is easy to *shift* some of the training instances (especially around the decision hyperplane) so that the dataset becomes linearly separable
- Doing this too much will change the train data significantly and we will not learn the concept expressed by our train data
- Try to minimise the amount of shifting we do for train instances to make the problem linearly separable
  - Each train instance is associated with a slack variable that is set to a non-zero value such that the corresponding training instance is moved sufficiently to the correct side of the decision hyperplane

SVMs and slack variables



$\xi_n > 1$ misclassification

$$t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n, \qquad n = 1, \ldots, N$$

slacked version of the constraint

$$C \sum_{n=1}^{N} \xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

objective function

C: cost-parameter
Higher values of C impose heavier penalties of slacking, whereas smaller C values will change the train data significantly. In practice use cross-validation to set C.

SVM slack version

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n \left\{t_n y(\mathbf{x}_n) - 1 + \xi_n\right\} - \sum_{n=1}^{N}\mu_n \xi_n$$

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)$$

$$\frac{\partial L}{\partial b} = 0 \quad \Rightarrow \quad \sum_{n=1}^{N} a_n t_n = 0$$

$$\frac{\partial L}{\partial \xi_n} = 0 \quad \Rightarrow \quad a_n = C - \mu_n.$$

$$\boxed{\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)}$$

Same Lagrangian as before!

SVM Implementations

- LIBSVM
  - http://www.csie.ntu.edu.tw/~cjlin/libsvm/
  - Available in a large number of programming languages
- SVM Light
  - http://svmlight.joachims.org/
  - can do ranking SVMs

Home Work

- Use LIBSVM to train a binary sentiment classifier using the train data provided in the Assignment 1
- Compare the performance with the perceptron classifier that you implemented