Intermediate Topics in Machine Learning & Deep Learning

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Schedule

Day 1

Session 1: Intermediate Topics in ML (SVMs and Kernels)
Session 2: Transfer Learning & Generating Labels for Deep Learning

Day 2

Session 3: Dimensionality Reduction and Variational Autoencoders (VAEs)
Session 4: Representation Learning, Weakly Supervised, Semi-supervised, and self-supervised learning

Support Vector Machines

- Method for supervised classification
  - Binary classification (two class)

- Generalization of *maximal margin classifier*
- *Support vector classifier*: can be applied to data that is not linearly separable
- *Support vector machine*: non-linear decision boundary

Maximal Margin Classifier

- *Maximal margin classifier*
  - Key assumption: two classes are separable by linear decision boundary

- First, we need to review *hyperplanes*…

Hyperplanes

- What is a hyperplane?
  - In d-dimensional space, a $(d-1)$-dimensional affine subspace
    - e.g. line in 2D, plane in 3D
  - Hyperplane in d-dimensional space:

$$(\star)\ \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_d x_d = 0$$

  - Separates space into two half-spaces

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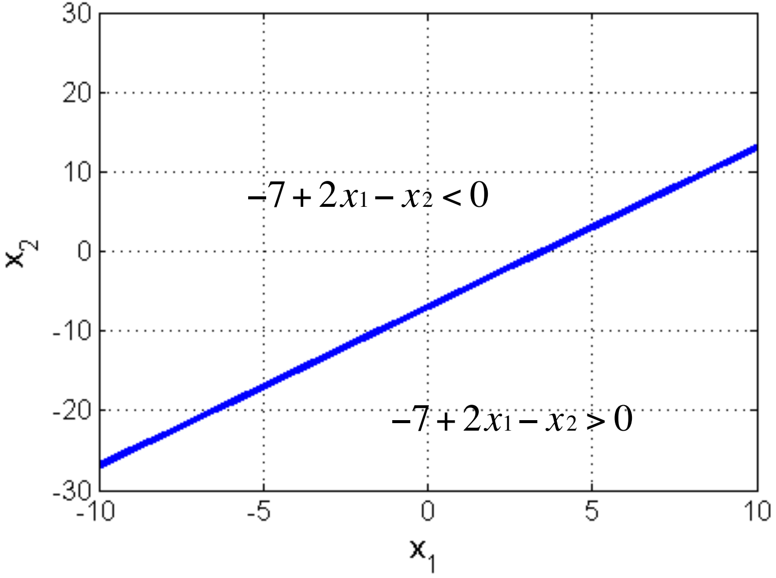
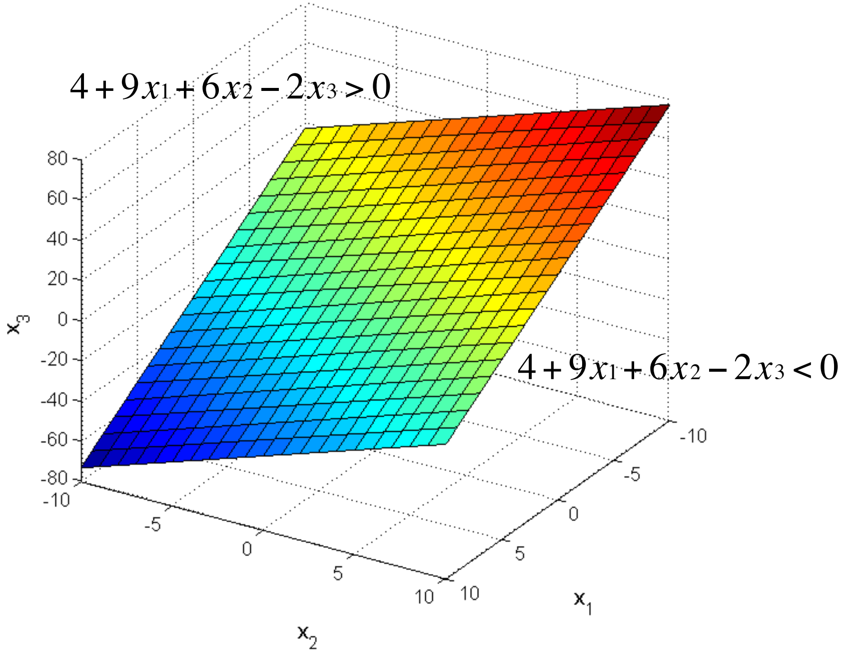
Hyperplanes

$$-7 + 2x_1 - x_2 = 0$$



$$4 + 9x_1 + 6x_2 - 2x_3 = 0$$



Separating Hyperplane Classifier

Idea:
Use a separating hyperplane for binary classification

Key assumption:
Classes can be separated by a linear decision boundary

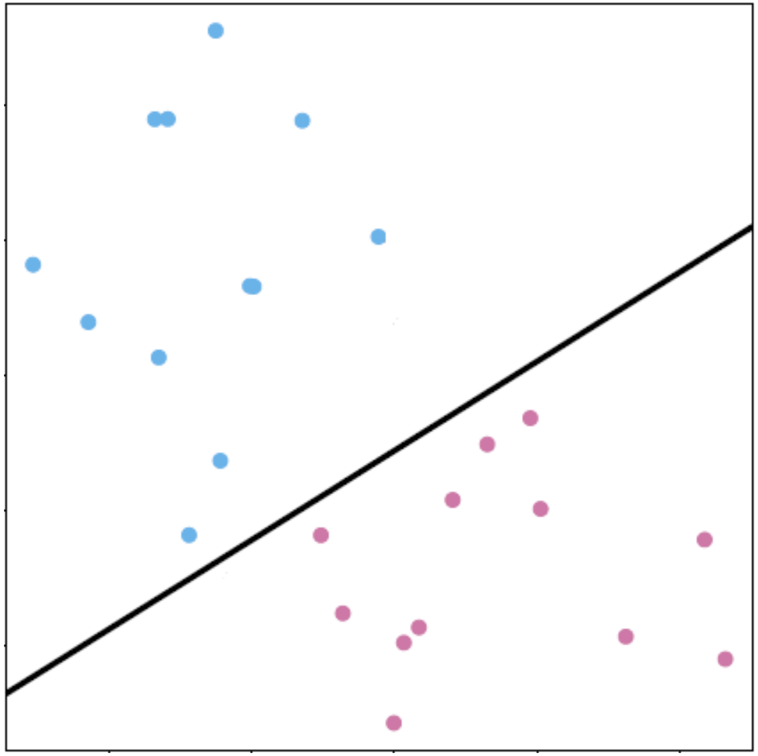


Figure 9.2 , ISL 2013

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Separating Hyperplane Classifier

To classify new data points:

Assign class by location of new data point with respect to hyperplane:

$$\hat{Y} = \text{sign}\left(\beta_0 + \beta_1 X_1 + \cdots + \beta_d X_d\right)$$

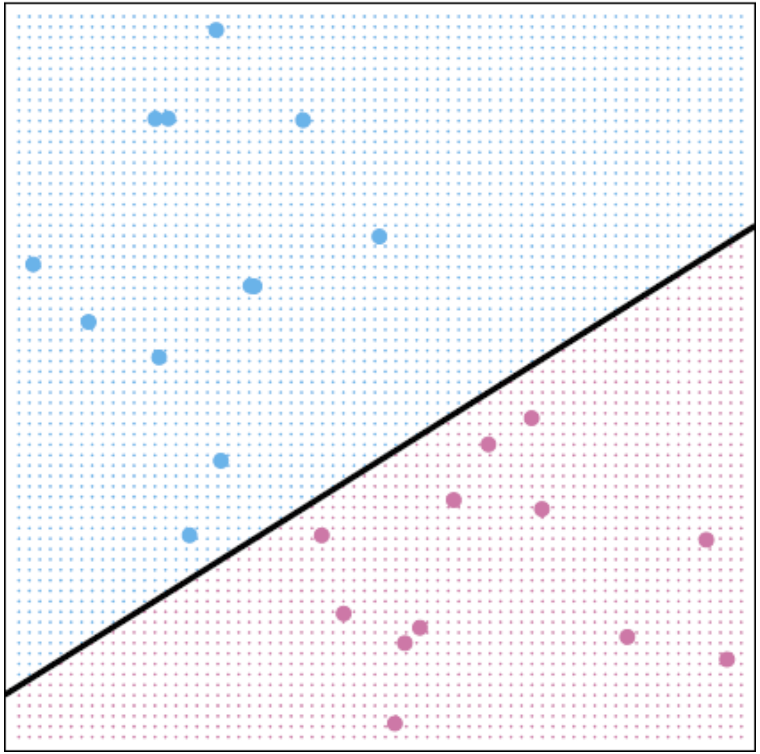

Figure 9.2 , ISL 2013

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Separating Hyperplane Classifier

Key assumption:
Classes can be separated by a linear decision boundary

→ Many possible separating hyperplanes…

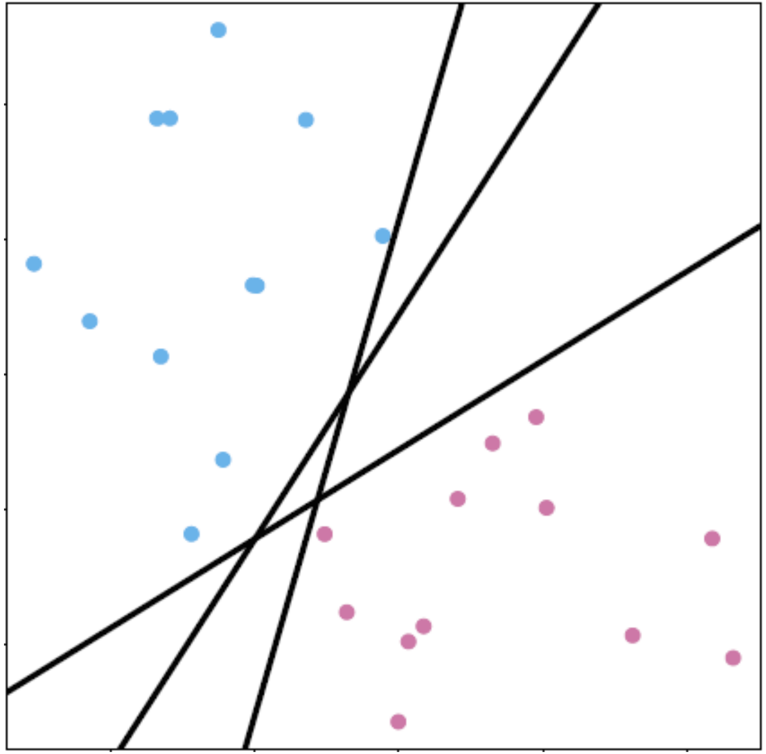

Figure 9.2 , ISL 2013

Mini Quiz:

Which linear decision boundary?

What criteria would you use to choose?

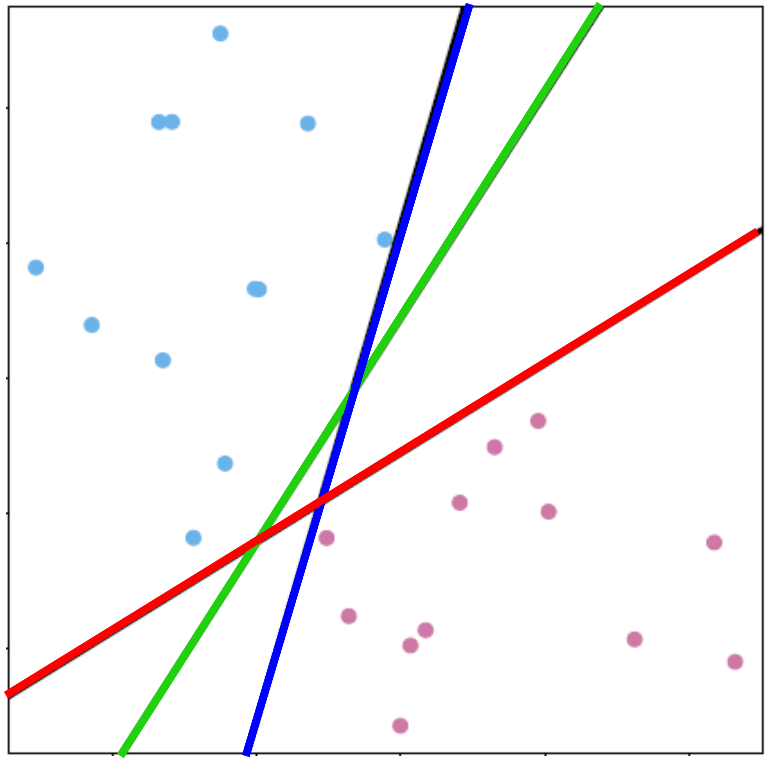

Figure 9.2 , ISL 2013

Separating Hyperplane Classifier

Which linear decision boundary?

Separating hyperplane "farthest" from training data

→ "Maximal Margin Classifier"

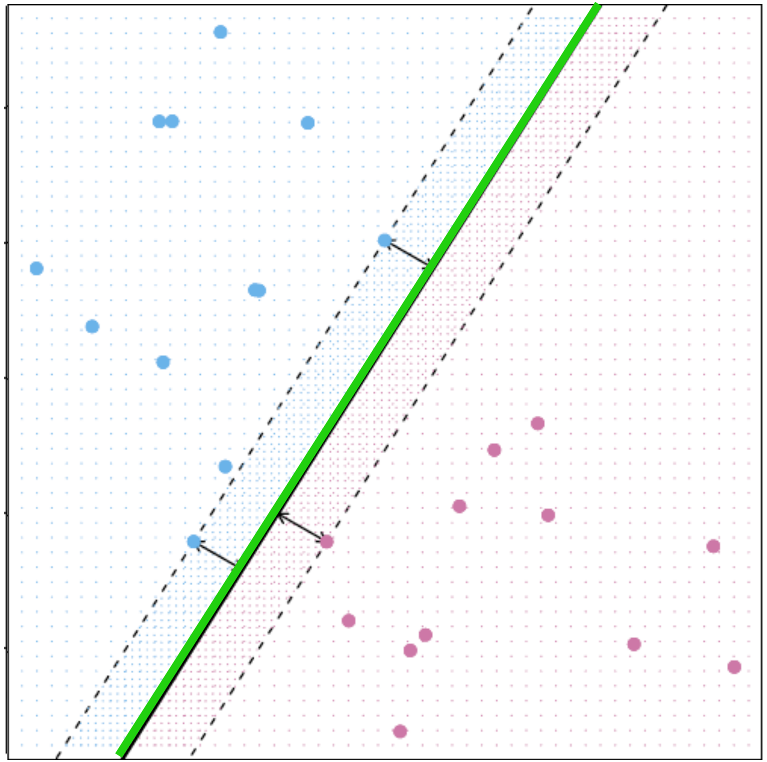

Figure 9.2, 9.3 , ISL 2013

Maximal Margin Classifier

Maximal margin hyperplane

Hyperplane “farthest” from training data → maximizes margin

Margin: smallest distance between any training observation and the hyperplane

Support vectors: the training observations equidistant from the hyperplane

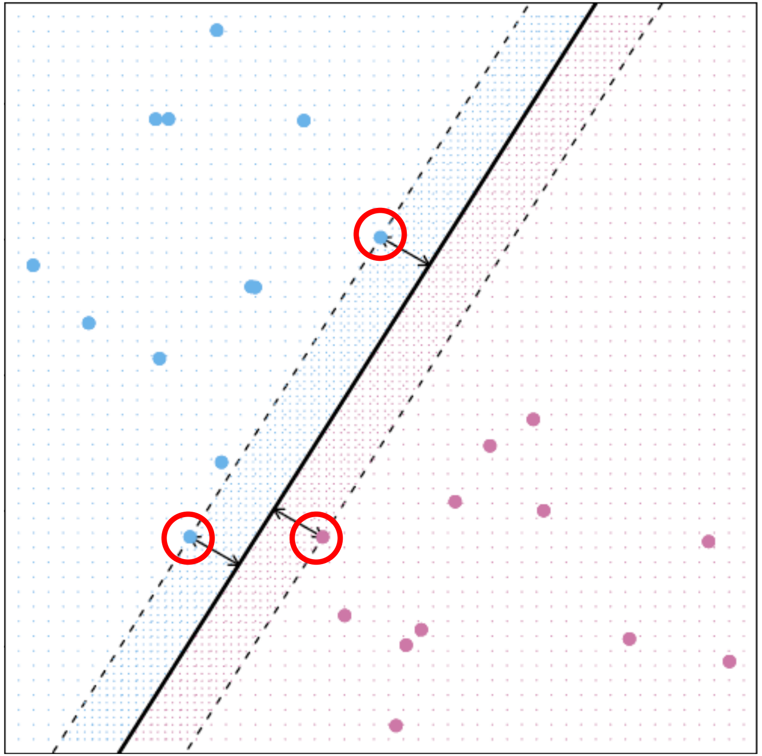

Figure 9.3 , ISL 2013

Maximal Margin Classifier

- *Support vectors*
  - The training observations equidistant from the maximal margin (MM) hyperplane
  - "Support": MM hyperplane only depends on these observations
    - If support vectors are perturbed, then MM hyperplane will change
    - If any other training observations are perturbed, MM hyperlane not effected

Maximal Margin Classifier

- To find maximal margin hyperplane, solve:

$$\underset{(\beta_0,\ldots,\beta_d)}{\text{maximize}} \quad M$$

maximize the margin, M

$$\text{subject to} \quad \sum_{j=0}^{d} \beta_j^2 = 1$$

constraint necessary for well-defined optimization problem

$$Y^{(i)}\left(\beta_0 + \beta_1 X_1^{(i)} + \cdots + \beta_d X_d^{(i)}\right) \geq M, \ \forall i$$

all training points must be distance at least M from hyperplane

$Y^{(i)} \in \{-1, 1\}$ are the class labels

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Maximal Margin Classifier

Recall our assumption:

Classes can be separated by a linear decision boundary

What if there's no separating hyperplane?

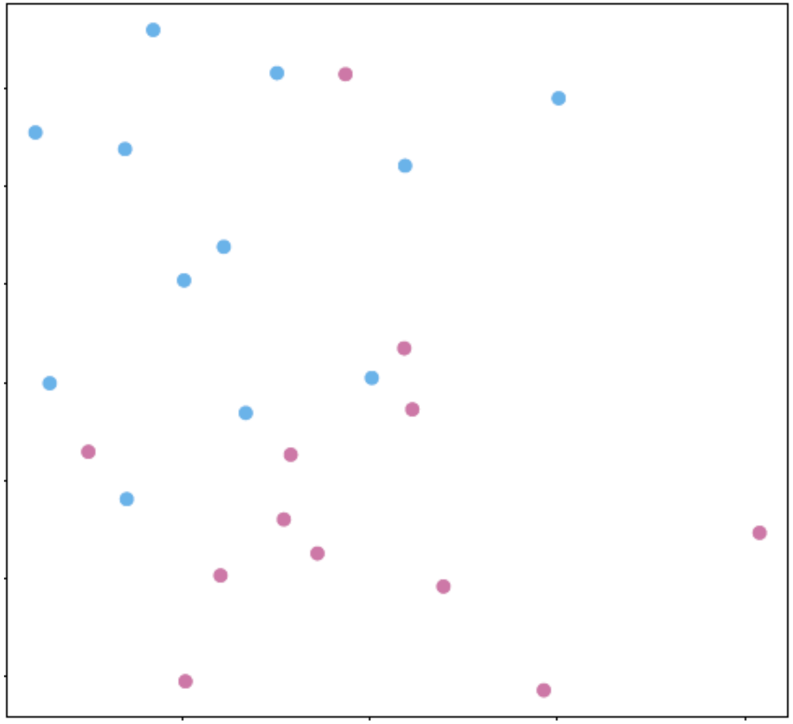

Figure 9.4 , ISL 2013

Maximal Margin Classifier

Disadvantage:

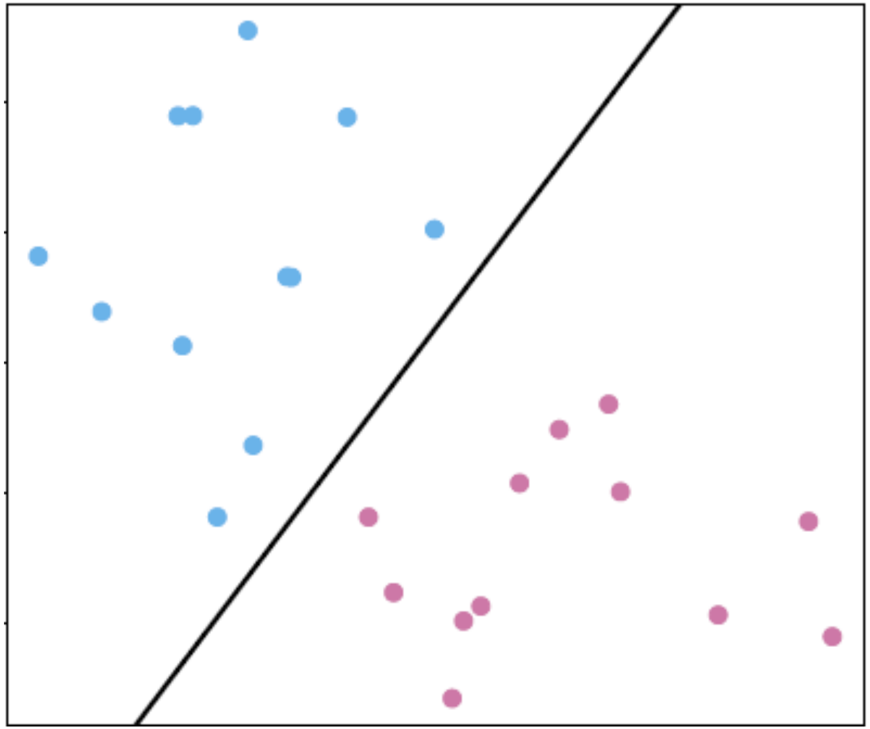

Figure 9.5 , ISL 2013

Maximal Margin Classifier

Disadvantage:

Can be sensitive to individual observations

May overfit training data

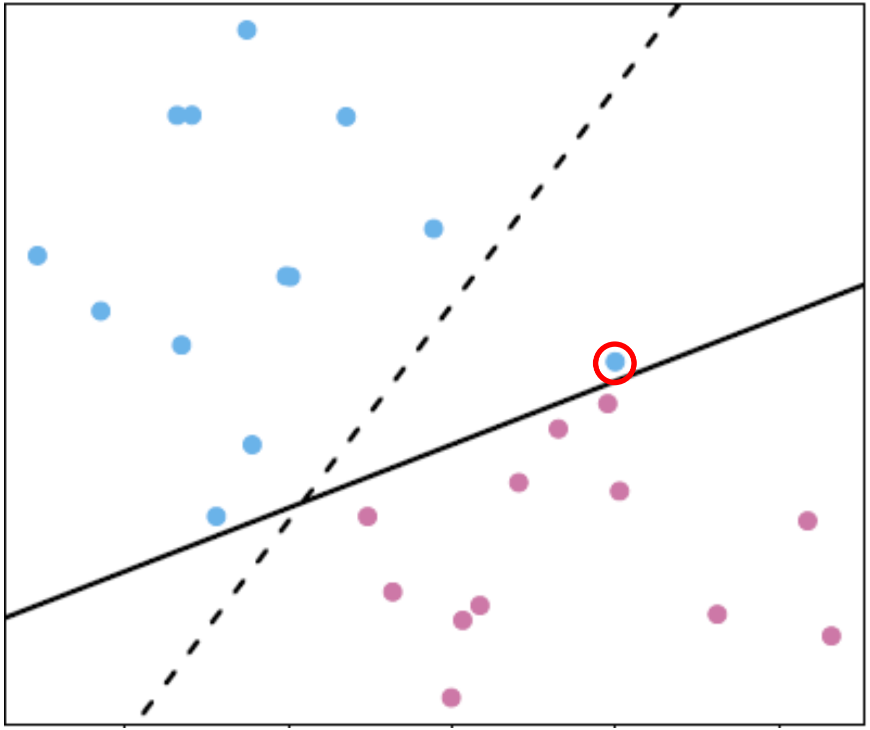

Figure 9.5 , ISL 2013

Support Vector Classifier

What if there’s no separating hyperplane?

Support Vector Classifier: allows training samples on the “wrong side” of the margin or hyperplane

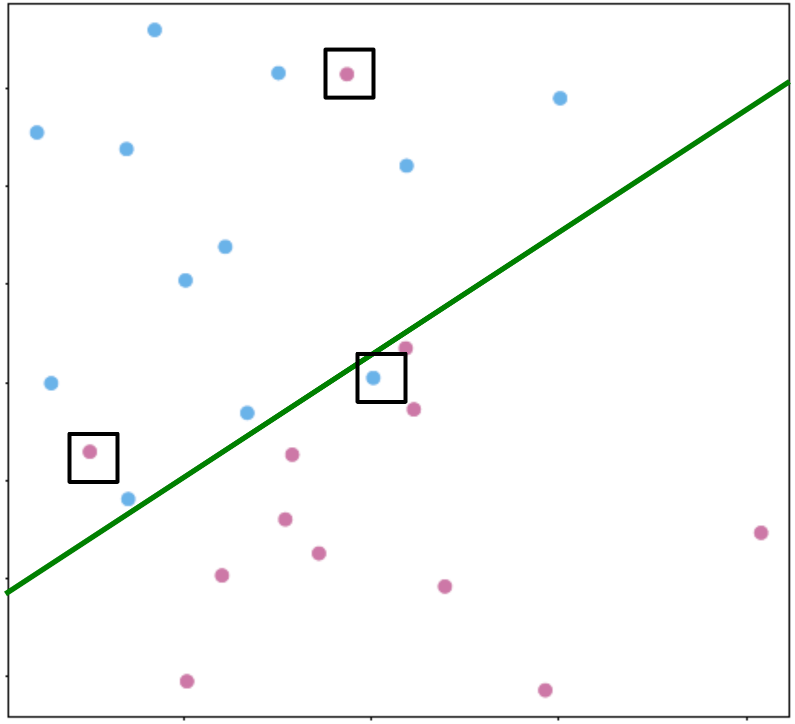

Figure 9.4 , ISL 2013

Support Vector Classifier

- *Support Vector Classifier*
  - Hyperplane-based classifier
  - Allows *some* training samples on "wrong side" of margin/hyperplane
  - *Soft margin*: margin is not a hard boundary

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Support Vector Classifier

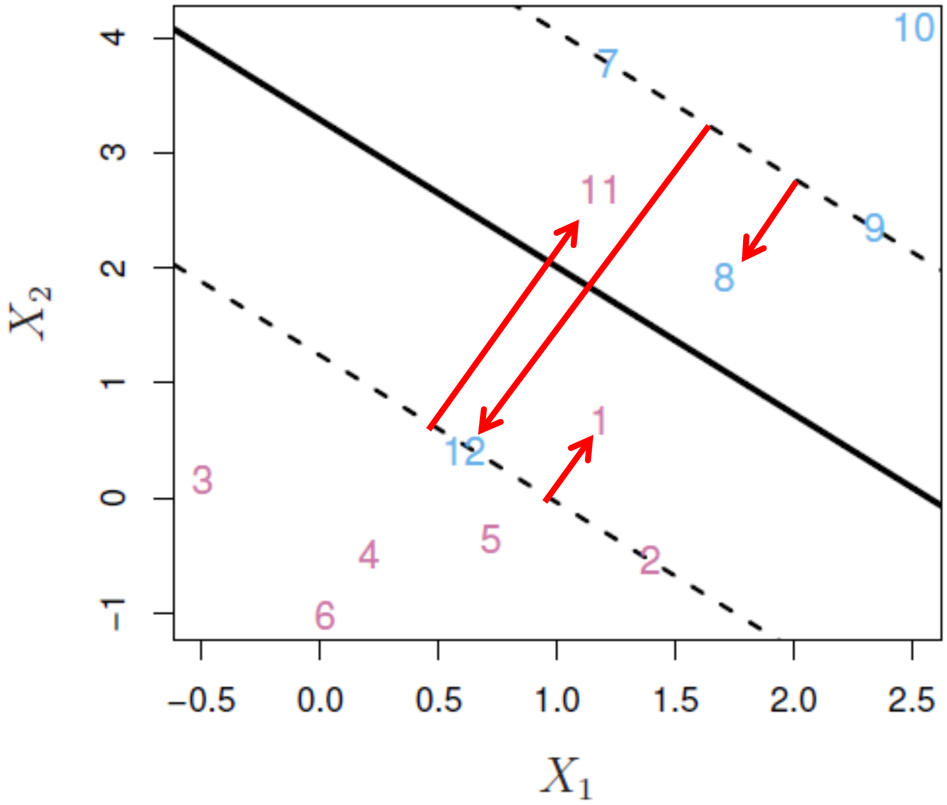

Figure 9.6 , ISL 2013

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Support Vector Classifier

- *Support Vector Classifier*
  - Hyperplane-based classifier
  - Allows *some* training samples on "wrong side" of margin/hyperplane
  - *Soft margin*: margin is not a hard boundary

- Idea: solve maximal margin problem, but allow violations of the margin
  - Impose penalty to limits number/degree of violations

Support Vector Classifier

- To find hyperplane for the SV classifier, solve:

maximize the margin, M

constraint necessary for well-defined optimization problem

training points less than distance M from hyperplane *pay a penalty ε_i*

$$\underset{(\beta_0,\ldots,\beta_d,\epsilon_1,\ldots,\epsilon_n)}{\text{maximize}} \quad M$$

$$\text{subject to} \quad \sum_{j=0}^{d} \beta_j^2 = 1$$

$$Y^{(i)}\left(\beta_0 + \beta_1 X_1^{(i)} + \cdots + \beta_d X_d^{(i)}\right) \geq M(1 - \epsilon_i),$$

$$\sum_{i=1}^{n} \epsilon_i \leq C, \qquad \epsilon_i \geq 0, \ \forall i$$

limit on total penalties

"slack" variable ε_i

Support Vector Classifier

- Slack variables ε_i allow for violations of the margin
  - $\varepsilon_i = 0$: training point $X^{(i)}$ is on correct side of margin
  - $\varepsilon_i > 0$: $X^{(i)}$ violates the margin
  - $\varepsilon_i > 1$: $X^{(i)}$ is misclassified (wrong side of hyperplane)

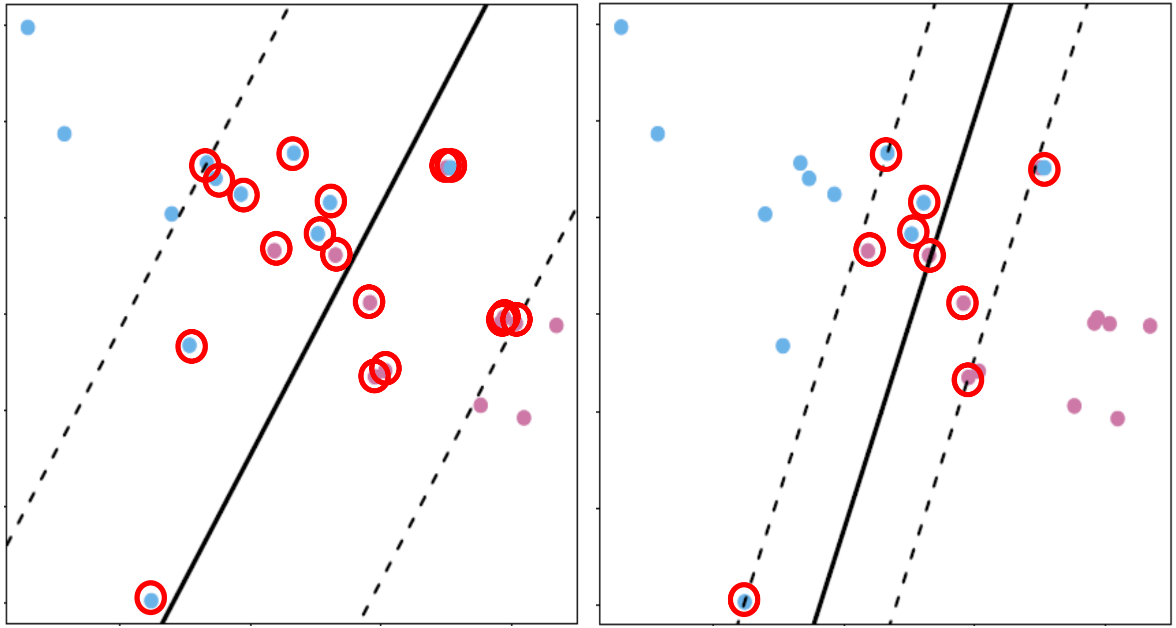
- Penalty parameter C – "budget" for violations
  - Allows at most C misclassifications on training set

Support Vector Classifier

"Misclassification budget" parameter C is selected by *cross-validation*

* controls bias-variance trade-off *

Support vectors: observations on margin or violating margin



Large budget
many Support Vectors

Small budget
fewer Support Vectors

Figure 9.7 , ISL 2013

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Support Vector Classifier

Disadvantage:

Linear decision boundary

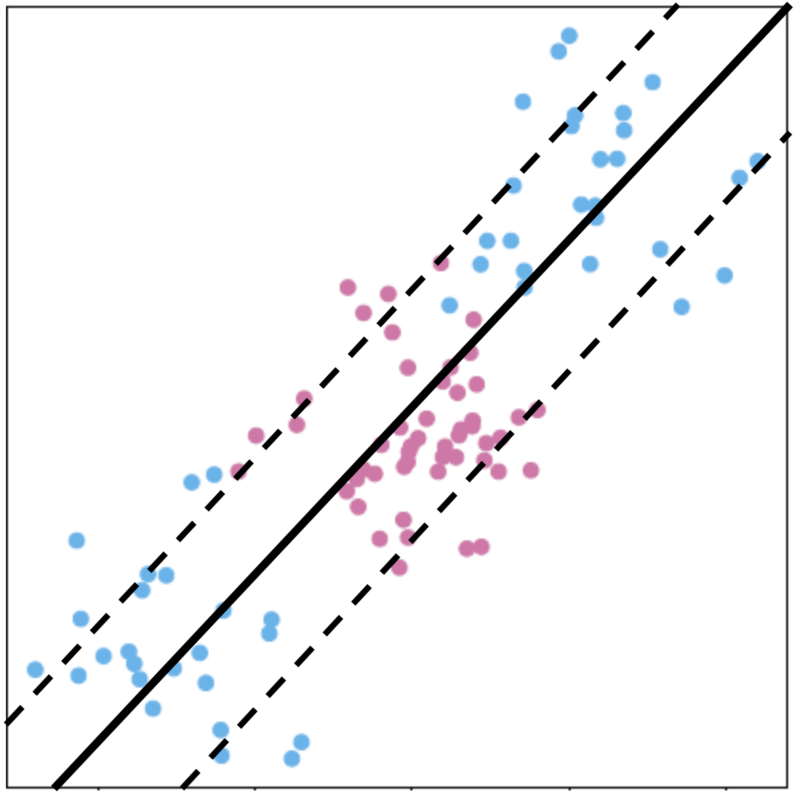
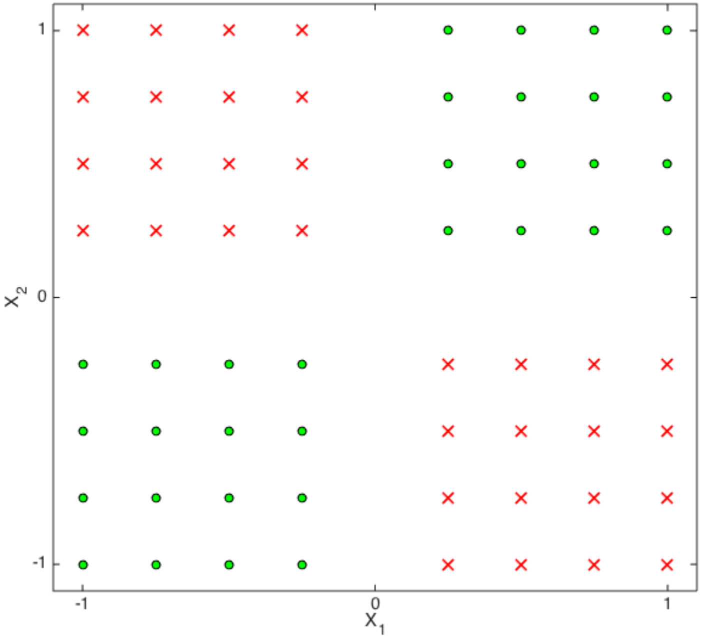


Figure 9.8 , ISL 2013

Expanding Feature Space



variables: X_1 , X_2

Some data sets are not linearly separable…

But they *become* linearly separable when transformed into a *higher* dimensional space

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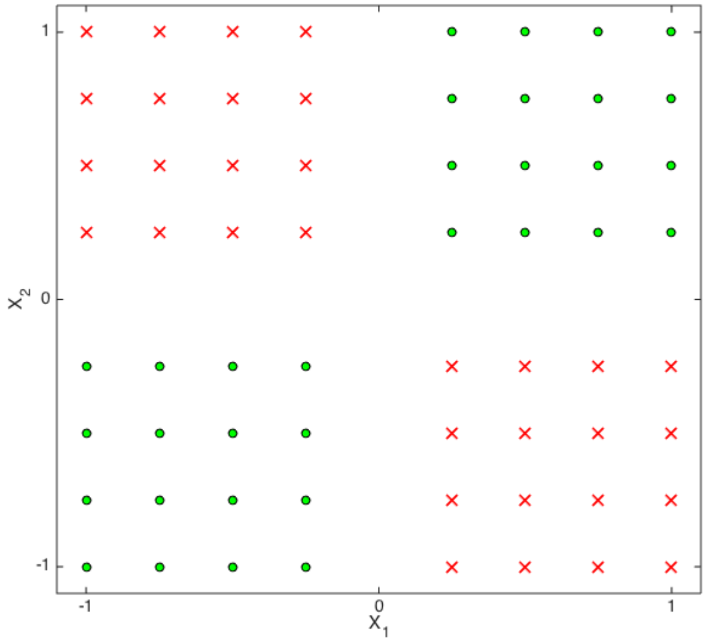
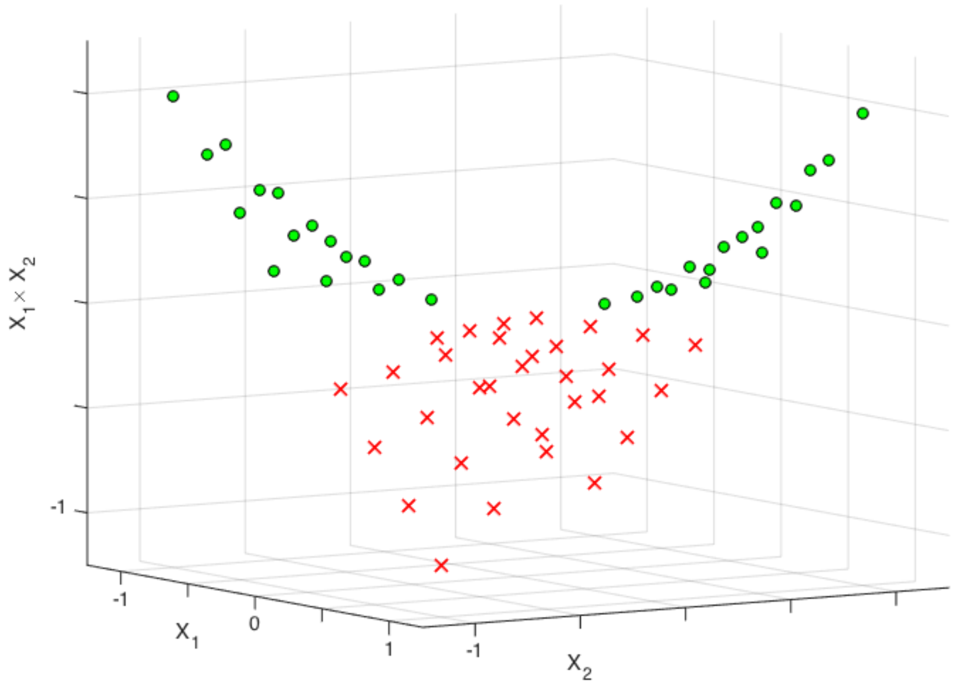
Expanding Feature Space



variables: X_1 , X_2



variables: X_1 , X_2, X_1X_2

Expanding Feature Space

- Linear regression → non-linear model
  - Create new features that are functions of predictors
- Apply same technique to support vector classifier
  - Consider polynomial functions of predictors:

Non-linear Decision Boundary

- Suppose our original data has d features:

$$X = [X_1, X_2, \cdots, X_d]$$

- Expand feature space to include 2d features:

$$\tilde{X} = [\underbrace{X_1}_{\tilde{X}_1}, \underbrace{(X_1)^2}_{\tilde{X}_2}, \underbrace{X_2}_{\tilde{X}_3}, \underbrace{(X_2)^2}_{\tilde{X}_4}, \cdots, \underbrace{X_d}_{\tilde{X}_{2d-1}}, \underbrace{(X_d)^2}_{\tilde{X}_{2d}}]$$

  – Decision boundary will be non-linear in original feature space

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Non-linear decision boundary

- Decision boundary in enlarged features space is linear:

$$\beta_0 + \beta_1 \tilde{X}_1 + \beta_2 \tilde{X}_2 + \cdots + \beta_{2d-1} \tilde{X}_{2d-1} + \beta_{2d} \tilde{X}_{2d} = 0$$

- Decision boundary in enlarged features space is an ellipse *in the original features space*:

$$\beta_0 + \beta_1 X_1 + \beta_2 (X_1)^2 + \cdots + \beta_{2d-1} X_d + \beta_{2d} (X_d)^2 = 0$$

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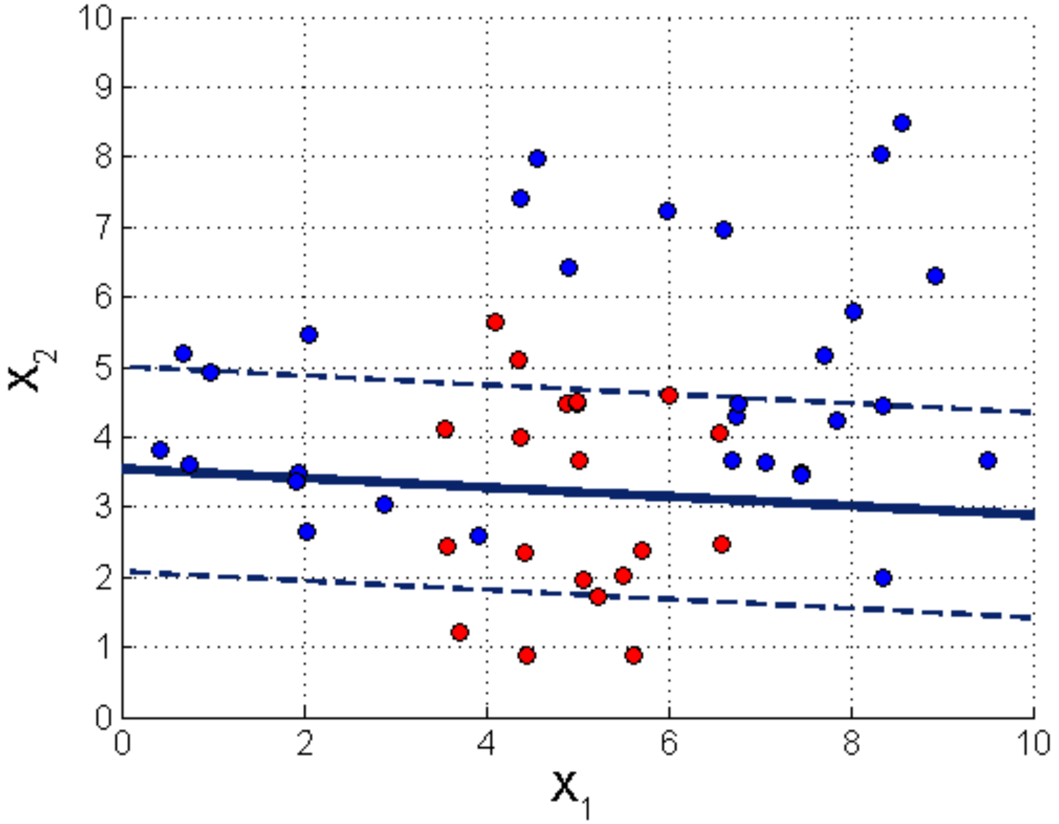
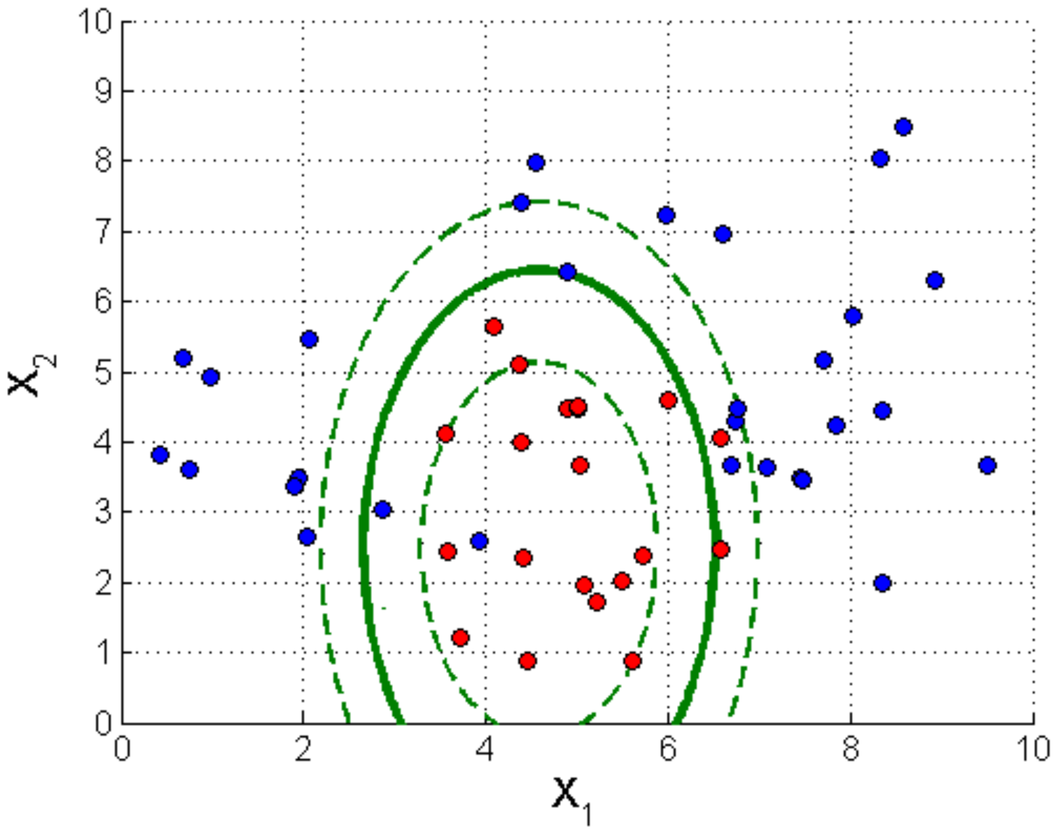
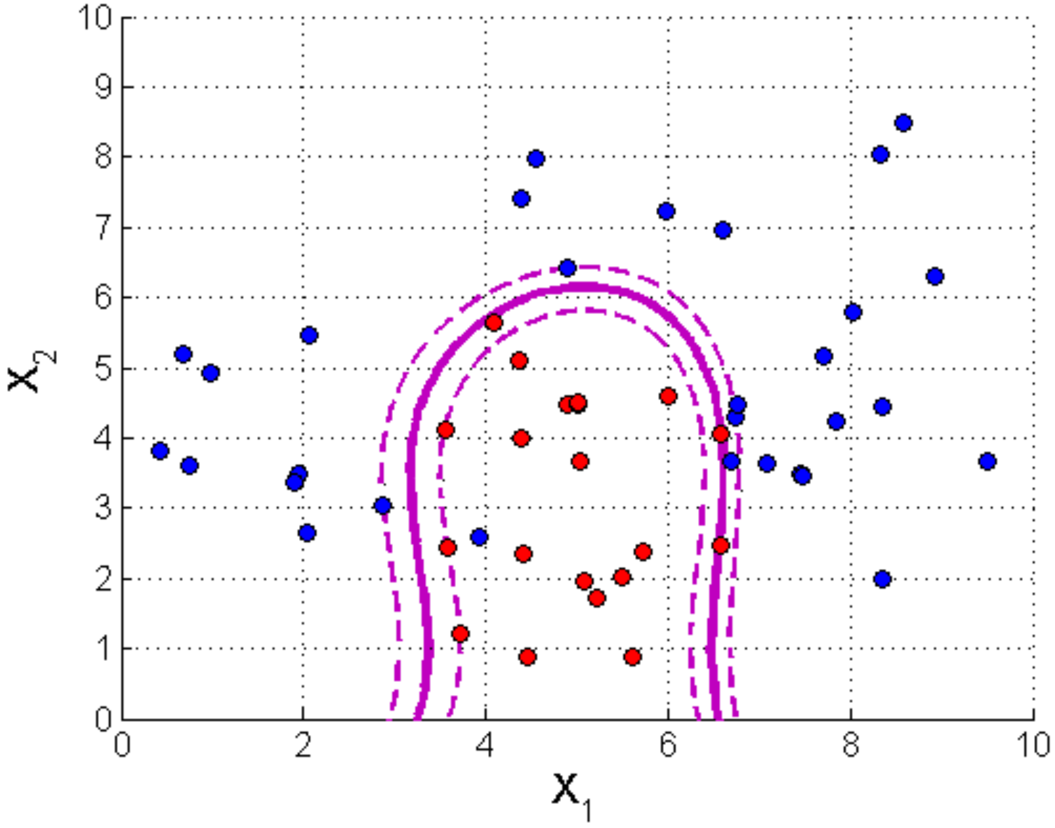
Non-linear Decision Boundary



Non-linear Decision Boundary



Non-linear Decision Boundary

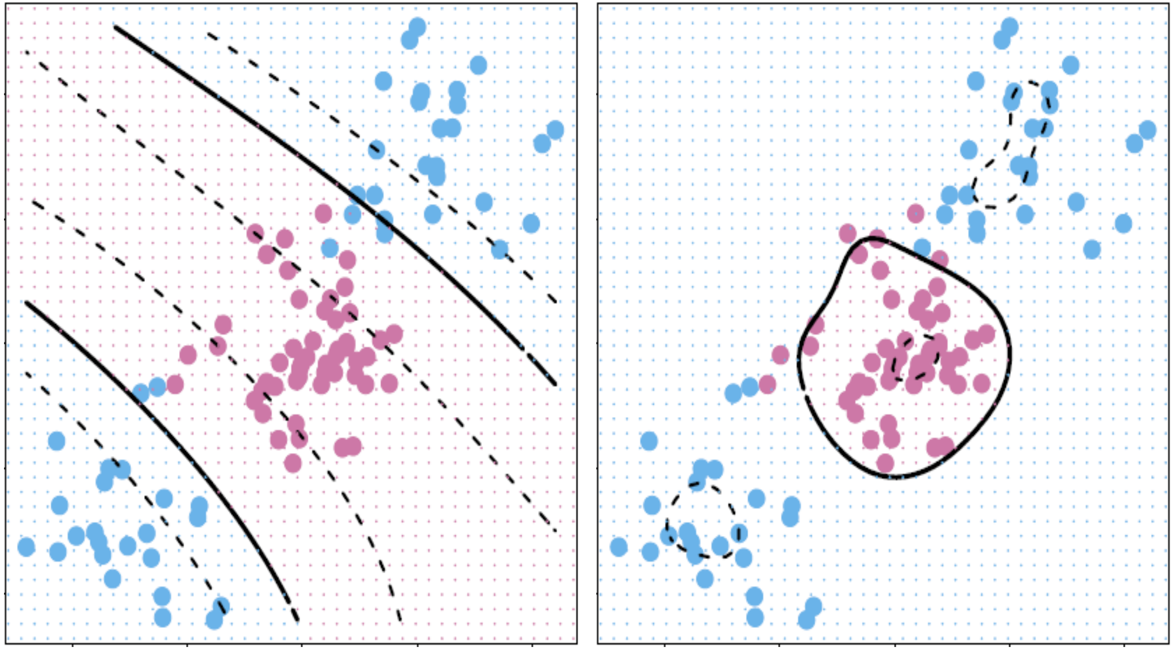


Non-linear Decision Boundary

- Add higher order polynomial terms to expanded features set → number of features grows quickly
  - Large number of features becomes computationally challenging
  - We need an efficient way to work with large number of features

Support Vector Machine (SVM)

Support Vector Machine: extension that uses *kernels* to achieve *non-linear decision boundary*



Support Vector Machine

- *Kernel*: generalization of inner product

- Kernels (implicitly) map data into higher-dimensional space
  - Apply support vector classifier in high-dimensional space with hyperplane (linear) decision boundary

Support Vector Machine

- Computations in support vector classifier requires only inner products of training data

$$f(X) = \beta + \sum_{i \in S} \alpha_i \langle X^{(i)}, X \rangle$$

- In SVM we replace inner product with kernel function

$$f(X) = \beta + \sum_{i \in S} \alpha_i K\left(X^{(i)}, X\right)$$

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Support Vector Machine

- Properties of kernels $K(X, X')$:
  - Generalization of inner product

$$K(X, X') = \langle \phi(X), \phi(X') \rangle, \quad \phi \text{ feature mapping}$$

  - Symmetric: $K(X, X') = K(X', X)$
  - Gives a measure of similarity between X and X'
    - If X and X' close together, then $K(X, X')$ large
    - If X and X' far apart, then $K(X, X')$ small

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Support Vector Machine

- Linear kernel

$$K(X, X') = \langle X, X' \rangle$$

- Polynomial kernel (degree p)

$$K(X, X') = (1 + \langle X, X' \rangle)^p$$

- Radial basis kernel

$$K(X, X') = \exp\left(-\gamma \|X - X'\|^2\right)$$

Support Vector Machine

- Why use kernels instead of explicitly constructing larger feature space?
  - Computational advantage

$$\phi : \mathbb{R}^d \to \mathbb{R}^D, \quad d << D$$

$$K(X, X') = \langle \phi(X), \phi(X') \rangle \quad \text{in } O(d)$$

- Other machine learning methods use kernels
  - e.g. kernel PCA

- Example: polynomial kernel, p = 2, d = 2:

$$K(X,Y) = (1 + \langle X, Y\rangle)^2 \qquad X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

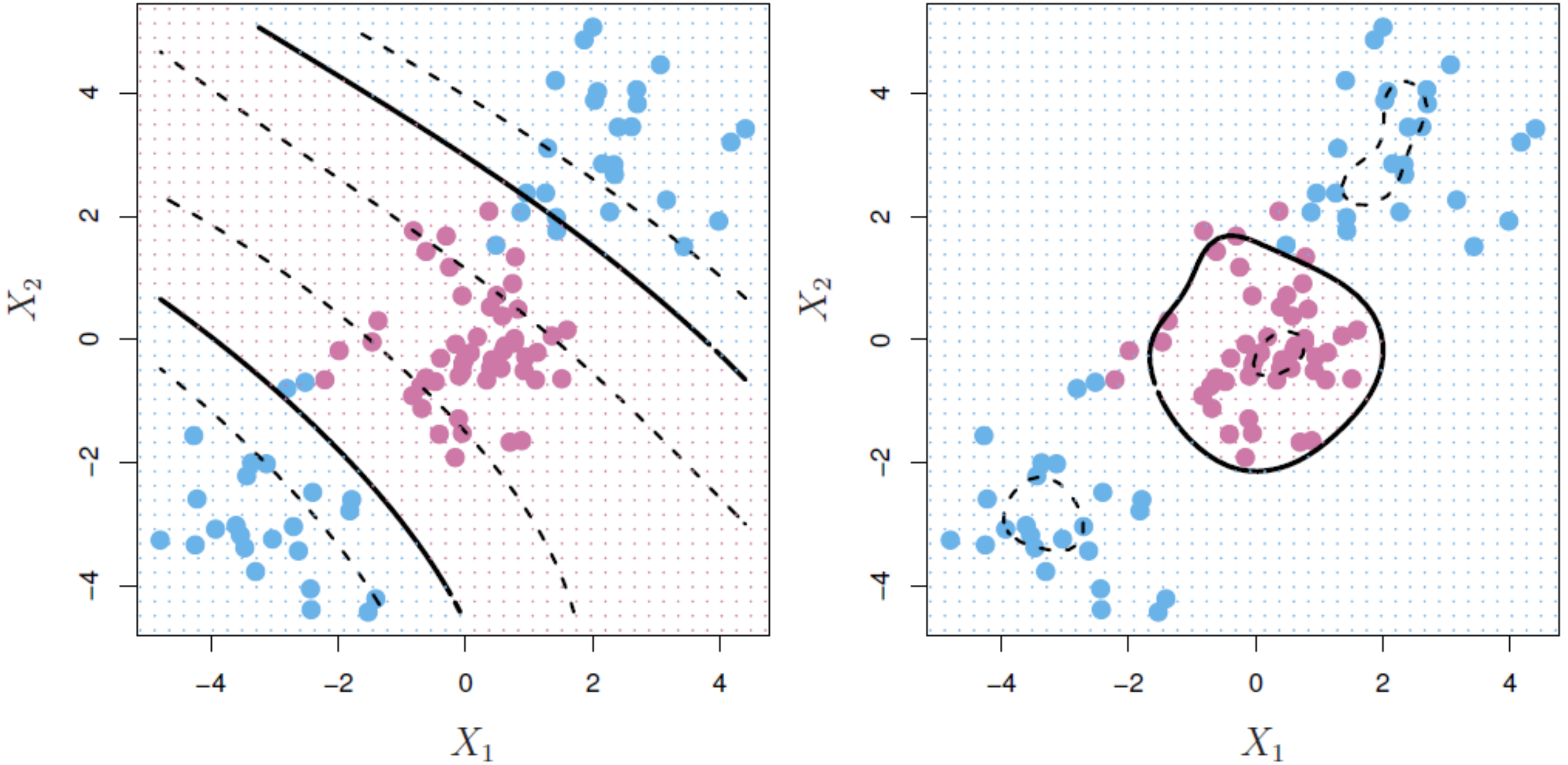
Then

$$K(X,Y) = 1 + 2X_1Y_1 + 2X_2Y_2 + X_1^2Y_1^2 + X_2^2Y_2^2 + 2X_1Y_1X_2Y_2$$

$$= \langle \phi(X), \phi(Y)\rangle$$

$$\text{where} \quad \phi(X) = \begin{bmatrix} 1 \\ \sqrt{2}X_1 \\ \sqrt{2}X_2 \\ \sqrt{2}X_1X_2 \\ X_1^2 \\ X_2^2 \end{bmatrix}$$

Support Vector Machine



Support Vector Machine

- Advantages
  - Regularization parameter C to avoid overfitting
  - Use of kernel gives flexibility in form of decision boundary
  - Optimization problem convex – unique solution

- Disadvantages
  - Must tune hyperparameters (e.g. C, kernel function)
    - Poor performance if not well-chosen
  - Must formulate as binary classification
  - Difficult to interpret

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Questions?

SVM with 3+ classes

- SVMs are designed for binary classification
  - Separating hyperplane naturally separates data into two classes
- How do we handle the case when the data belong to more than two classes?
- Popular approaches:
  1. One-versus-one
  2. One-versus-all

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SVM with 3+ classes

- *One-versus-one* classification
  - Construct an SVM for each pair of classes
  - For K classes, this requires training $\frac{K(K-1)}{2}$ SVMs
  - To classify a new observation, apply all $\frac{K(K-1)}{2}$ SVMs to the observation – take the most frequent class among pairwise results as predicted class
  - Disadvantage: computationally expensive for large values of K

SVM with 3+ classes

- *One-versus-all* classification
  - Fit K SVMs, in which class k represents one class, and the remaining $K - 1$ classes are combined to form the second class
  - Distance to separating hyperplane is a proxy for confidence of the classification
  - For new observation, choose "highest confidence" class to make prediction

Questions?

Imbalanced Classes

- Imbalanced classes: one class (+) occurs significantly more frequently in training set than the other (–)
  - e.g. fraud detection, medical database

- Why is this a problem?
  - Algorithms perform best when trained on roughly even numbers of observations in each class
  - Poor performance on underrepresented class

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Imbalanced Classes

- How can we improve performance when we have imbalanced classes?
  - Collect more data for underrepresented class
  - Weighting of classes
  - Sampling methods

Imbalanced Classes

- Weighting of classes: applying different weights to false negatives in cost function
  - e.g. in SVM, larger weights to penalties for violations of margin for class $(-)$ than for class $(+)$:

$$\sum_{i=1}^{n} \epsilon_i < C \quad \text{becomes}$$

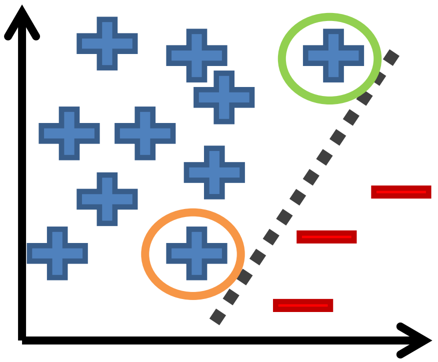
$$\left(\sum_{i:\, Y^{(i)}=(+)} \epsilon_i \right) + \omega \left(\sum_{i:\, Y^{(i)}=(-)} \epsilon_i \right) < C$$

Imbalanced Classes

- Sampling Methods – modify set of training observations to make classes more even
- Balance class labels by
  - Undersampling class (+)
  - Oversampling class (–)

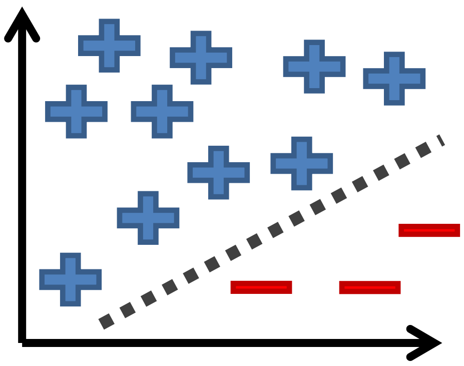
Imbalanced Classes

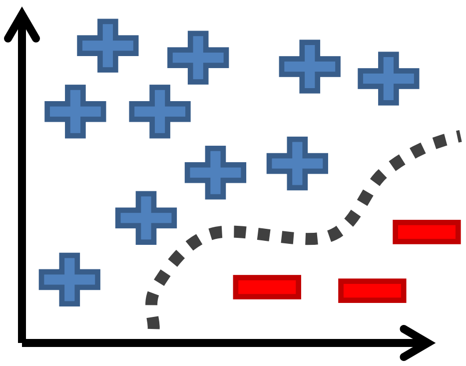
- Disadvantages of over/under sampling
  - Undersampling class (+) may remove important training observations



Imbalanced Classes

- Disadvantages of over/under sampling
  - Oversampling class (–) may result in over fitting





Imbalanced Classes

- Synthetic Minority Oversampling
  - Method for oversampling class $(-)$ that generates new minority observations by perturbing existing minority observations:

1. Selects observation $X^{(-)}$ in class $(-)$ at random
2. Finds k nearest neighbors of $X^{(-)}$ selects one of the neighbors $X_{nn}^{(-)}$ at random
3. New sample $X_{new}^{(-)}$ is a perturbation of $X^{(-)}$ along the direction $X_{nn}^{(-)} - X^{(-)}$

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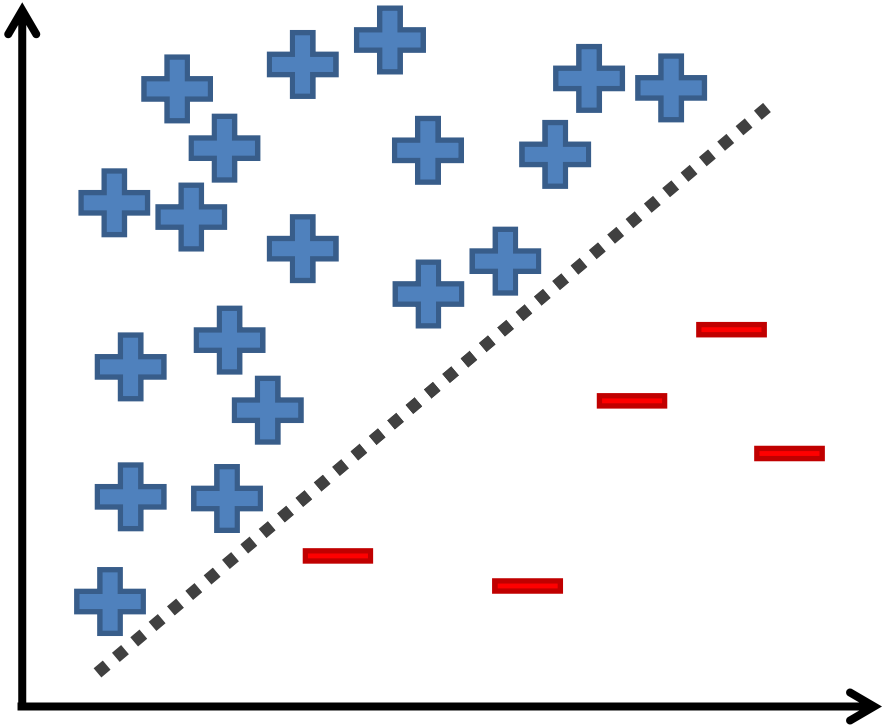
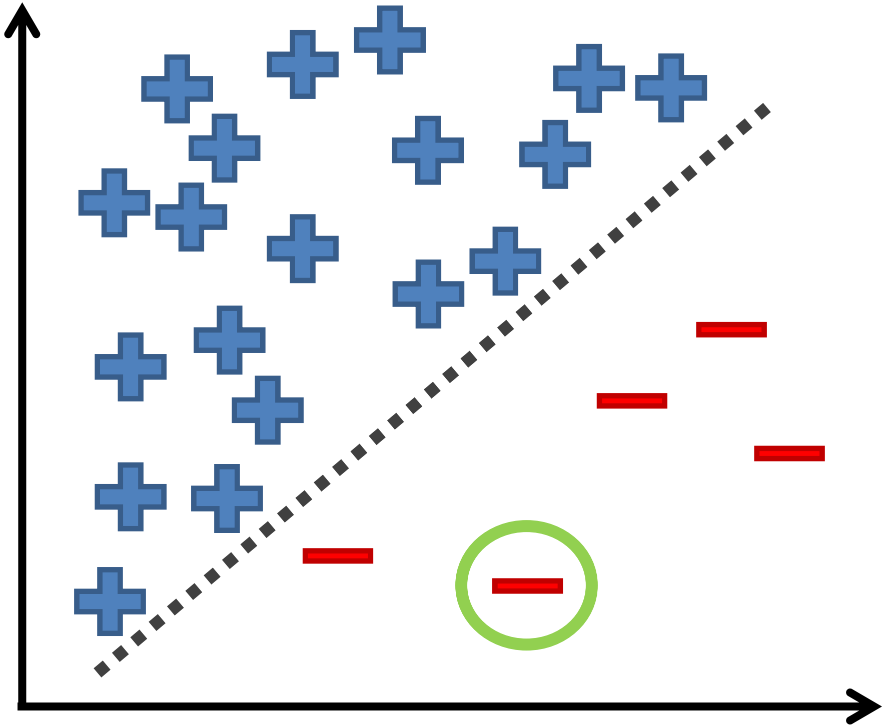
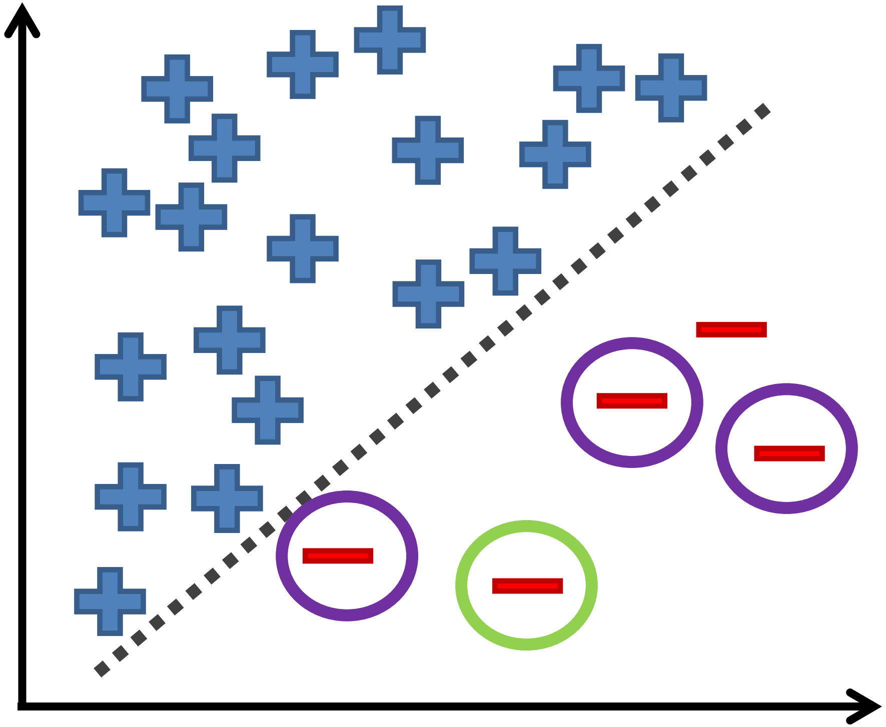
Imbalanced Classes



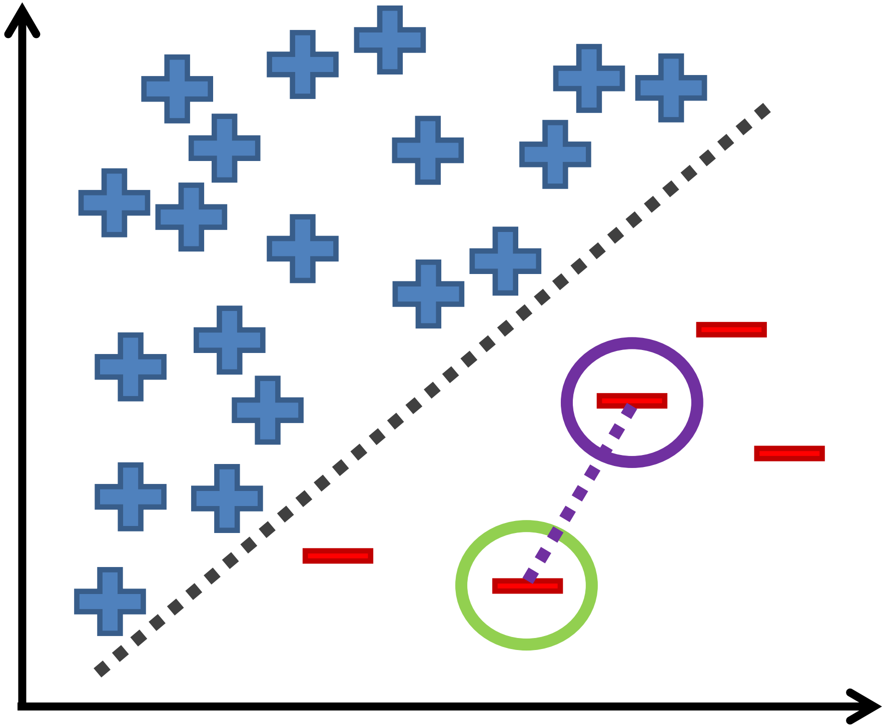
Imbalanced Classes



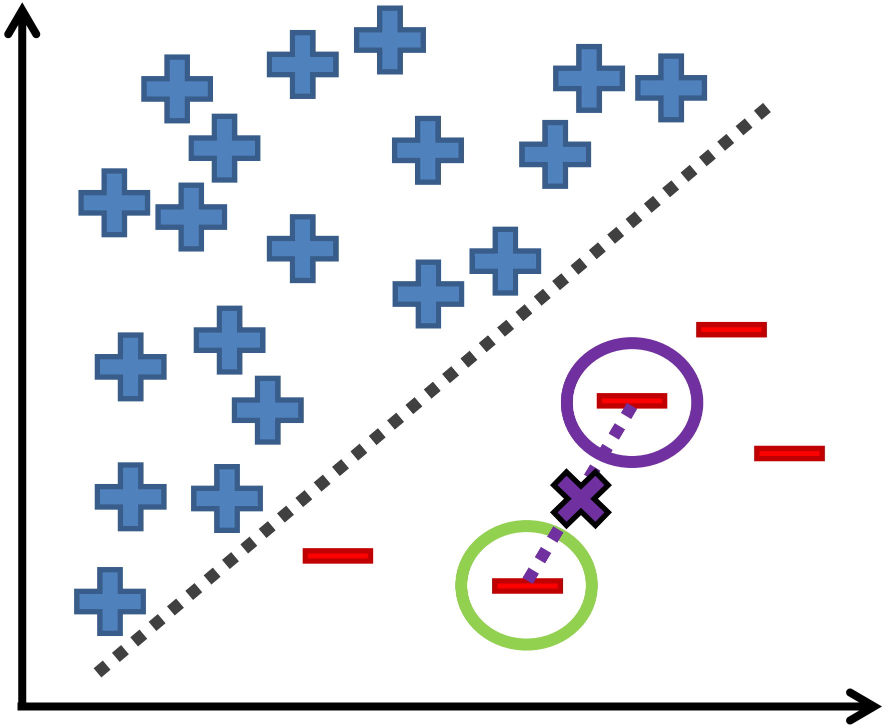
Imbalanced Classes



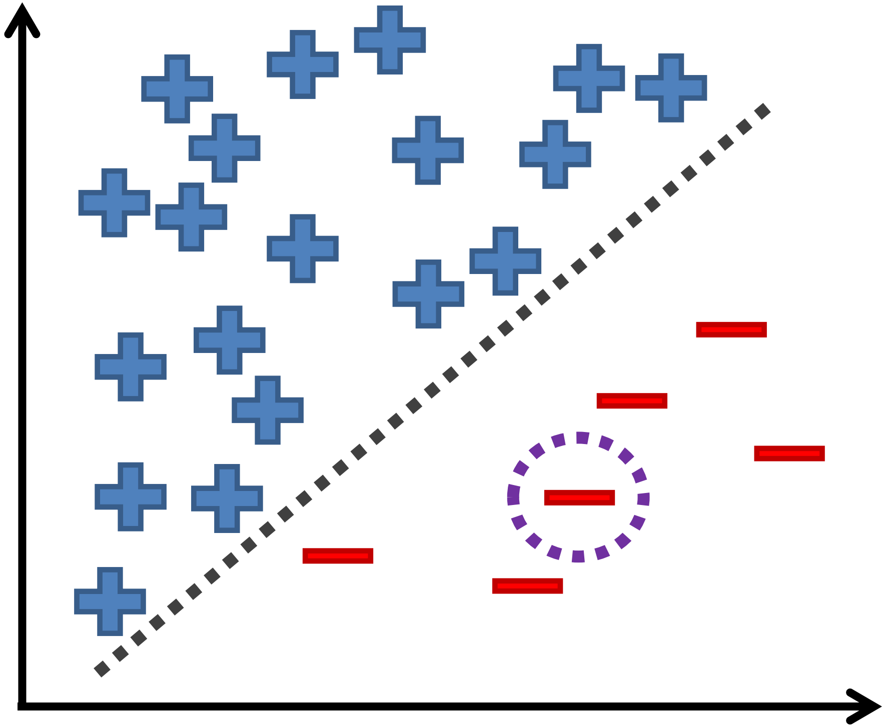
Imbalanced Classes



Imbalanced Classes



Imbalanced Classes



Measuring Classifier Performance

- In regression, we can use a criterion such as the residual sum of squares to measure error
- For classification, we need a measure of performance
  - Examples: Confusion matrix, Precision/Recall, Sensitivity/Specificity, ROC curve
- Consider binary classification with classes: (+) and (–)

Measuring Classifier Performance

- We can show the performance of the classifier in a table called a *confusion matrix*:
  - "Good performance": TP, TN large and FP, FN small

		Predicted class: +	Predicted class: –
True class	**+**	True Positive (TP)	False Negative (FN) Type II error
	–	False positive (FP) Type I error	True Negative (TN)

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Measuring Classifier Performance

True positive rate (TPR)

(recall, sensitivity)

True class \ Predicted class	+	−
+	**TP**	**FN**
−	FP	TN

$$TPR = \frac{TP}{TP + FN}$$

Positive predictive value (PPV) *(precision)*

True class \ Predicted class	+	−
+	**TP**	FN
−	**FP**	TN

$$PPV = \frac{TP}{TP + FP}$$

False positive rate (FPR)

True class \ Predicted class	+	−
+	TP	FN
−	**FP**	**TN**

$$FPR = \frac{FP}{FP + TN}$$

True negative rate (SPC)

(specificity)

True class \ Predicted class	+	−
+	TP	FN
−	**FP**	**TN**

$$SPC = \frac{TN}{FP + TN}$$

Measuring Classifier Performance

Precision/recall

ROC curve

True positive rate (TPR)

(recall, sensitivity)

Predicted class

True class	+	−
+	**TP**	**FN**
−	FP	TN

$$TPR = \frac{TP}{TP + FN}$$

Positive predictive value (PPV) *(precision)*

Predicted class

True class	+	−
+	**TP**	FN
−	**FP**	TN

$$PPV = \frac{TP}{TP + FP}$$

False positive rate (FPR)

Predicted class

True class	+	−
+	TP	FN
−	**FP**	**TN**

$$FPR = \frac{FP}{FP + TN}$$

True negative rate (SPC)

(specificity)

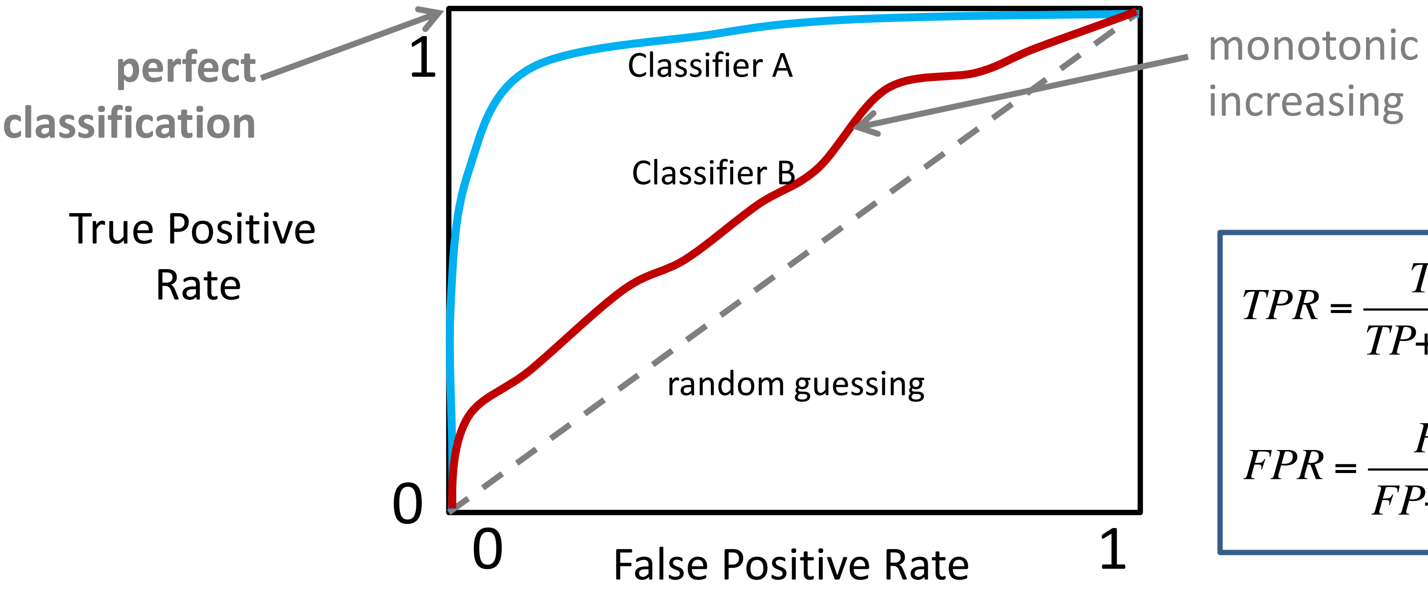
Predicted class

True class	+	−
+	TP	FN
−	**FP**	**TN**

$$SPC = \frac{TN}{FP + TN}$$

Measuring Classifier Performance

- ROC (receiver operating characteristic) curve



$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$

Measuring Classifier Performance

- Disadvantage of ROC curve - imbalanced classes
  - 1% samples belong to class “+” and 99% to class “–”
    - For results below then, TPR = **0.9**, FPR = **0.12** ← **looks good?**
    - TPR and FPR do not capture that **13x as many FP as TP**
    - *Alternative*: Precision = **0.07** (perfect: 1.0), Recall = TPR = **0.9**

		Predicted class	
		+	**–**
True class	**+**	**90**	10
	–	**1188**	8712

Measuring Classifier Performance

Precision / Recall

- Precision: fraction of samples predicted (+) that are actually (+)
- Recall *(true positive rate):* Fraction of (+) samples correctly predicted as (+)
- *Imbalanced class example*:
    - Precision = **0.07** (perfect: 1.0), Recall = TPR = **0.9** (perfect: 1.0)

True class	Predicted class +	Predicted class −
+	**90**	10
−	**1188**	8712

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Measuring Classifier Performance

- Precision/recall
  - Precision (Positive predictive value): $PPV = \frac{TP}{TP+FP}$
    - Fraction of samples predicted as (+) that are truly (+)
  - Recall (True positive rate): $TPR = \frac{TP}{TP+FN} = \frac{TP}{P}$
    - Fraction of (+) samples correctly classified as (+)
  - Recall and precision inversely related
  - In perfect classifier, Recall = 1, Precision = 1
  - Imbalanced class example: Recall = 0.9, Precision = 0.07

		Predicted class	
		+	**−**
True class	**+**	90	10
	−	1188	8712