Introduction to Classification

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Lecture 05.1.1 (v2.0.0)

Signposting

- We have wrapped up **classic statistics** with a discussion on non-parametrics, kernels, and a practical on missing data and outliers.
- The remainder of the course changes the focus towards machine-learning - especially the background of the key tools that are used in practice.
- It is important to emphasise that classification is statistics, though we use the parlance of machine learning.
  - Most of machine learning is also modern statistics.
  - The main distinction is about use: whether we use the results only for prediction, or for understanding.
  - Which ultimately is no distinction at all...

Intended Learning Outcomes

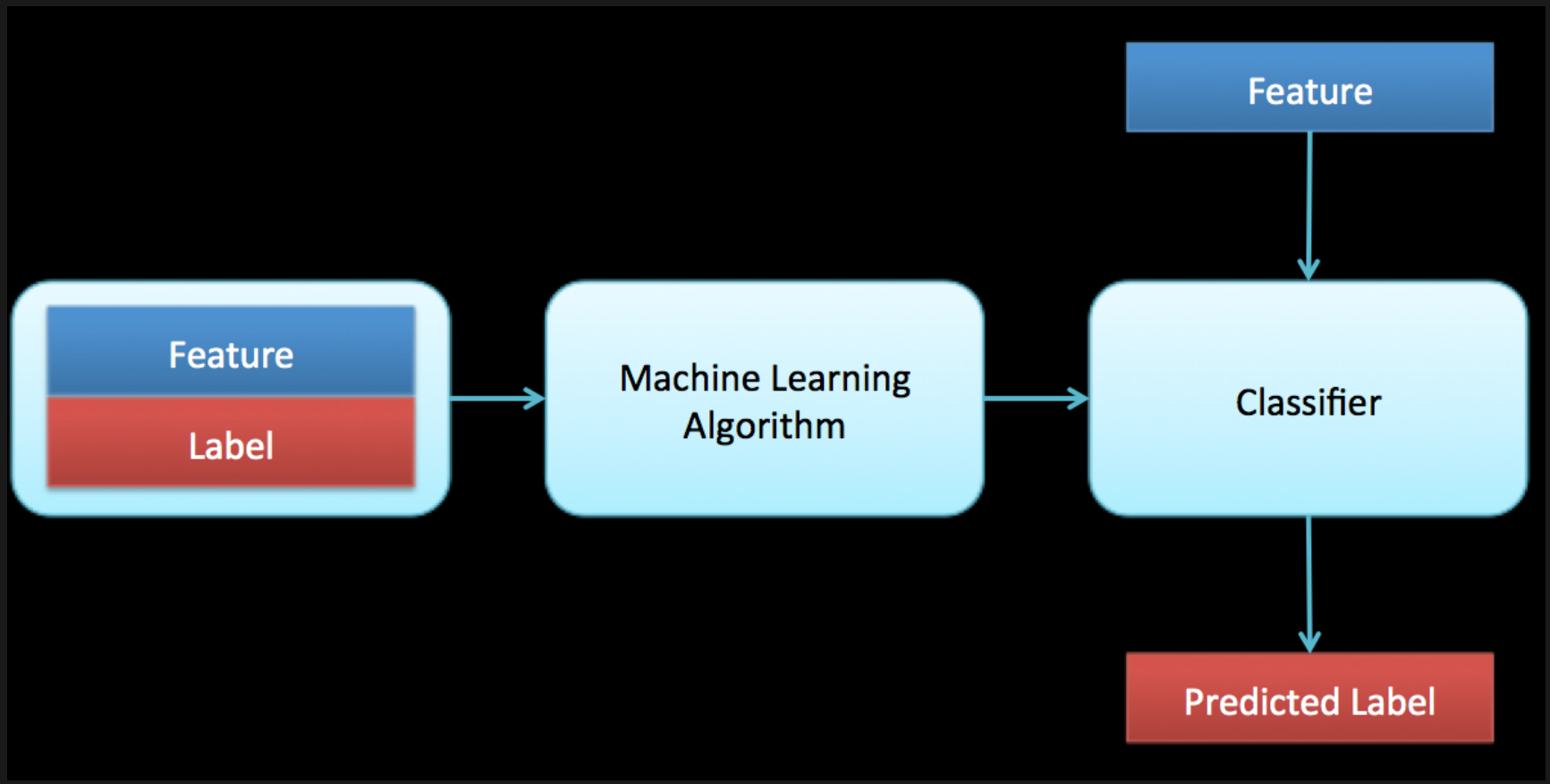
- ILO2 Be able to **use and apply basic machine learning** tools
- ILO3 Be able to make and report appropriate inferences from the results of applying basic tools to data

Types of machine learning

- Unsupervised: **no labels**. For example,
  - Clustering
  - Dimensionality reduction
  - Smoothing
- Supervised: exploits **labels**. For example,
  - Classification
  - Regression
- Other types:
  - Semi-supervised: **some labels** are available
  - Active: can **choose which labels** to obtain
  - Reinforcement: **reward based**. explore vs exploit?
  - etc.

Classification

- Machine Learning classification is about how to make good predictions of **classes** based on previous experience of how **features** relate to **classes**.



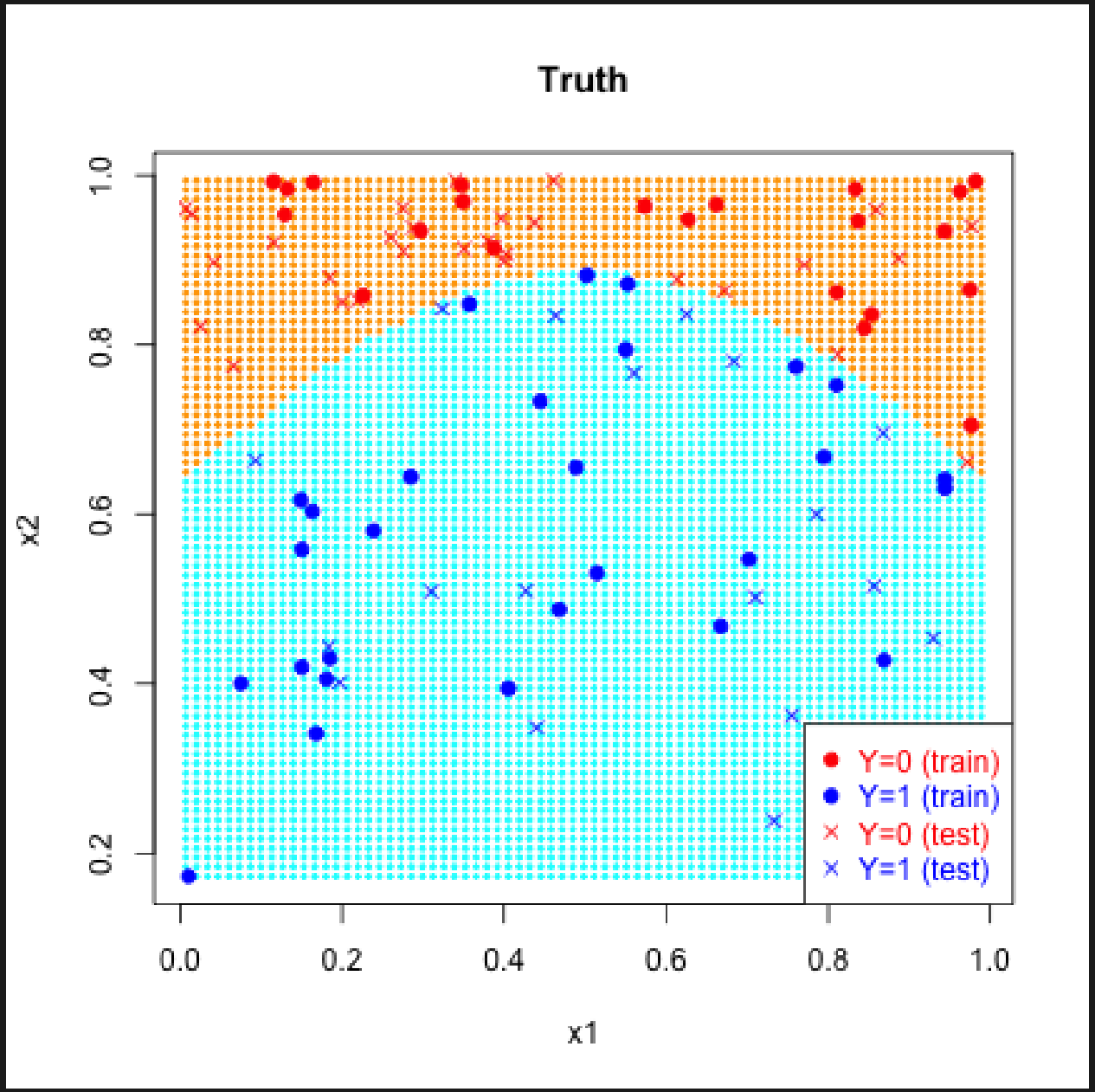
Examples of classification

- **Spam** filtering (spam/not spam)
- **Face detection** (image classification)
- **Speech recognition**
- **Handwriting recognition**
- **Turing test** . . . though that is human, not machine!
- In cyber:
  - **Malware detection** . . . when comparing to historical malware
  - **Intruder detection** . . . when comparing to intrusion models
- Classification is broadly the "detection, recognition, recall of **prior experience**".

Some Important Classifiers

- **Logistic Regression** (Block 2 and 5)
- **K-Nearest Neighbours** (Block 4 and 5)
- **Linear Discriminant Analysis** (Block 5)
- **Support Vector Machines** (Block 5)
- **Decision Trees** (Block 6)
- **CART**: Classification and Regression Trees (Block 6)
- **Random Forests** (Block 6)
- **Naive Bayes** (Block 7)
- **Neural Networks** (Block 9)

Classification



From Regression to Classification

- In Week 3 we discussed **linear regression**, i.e. obtaining solutions to:

$$y_i = \vec{x}_i \cdot \beta + e_i$$

- in scalar form, where we have p' covariates and have $\vec{x}_i = (1, x_{1,i}, \cdots, x_{p',i})$, so $\vec{x}_i$ and β are both vectors of length $p = p' + 1$, and e_i are the residuals whose squared-sum is minimised.
- Logistic regression instead solves for the probability that a binary outcome y is 1:

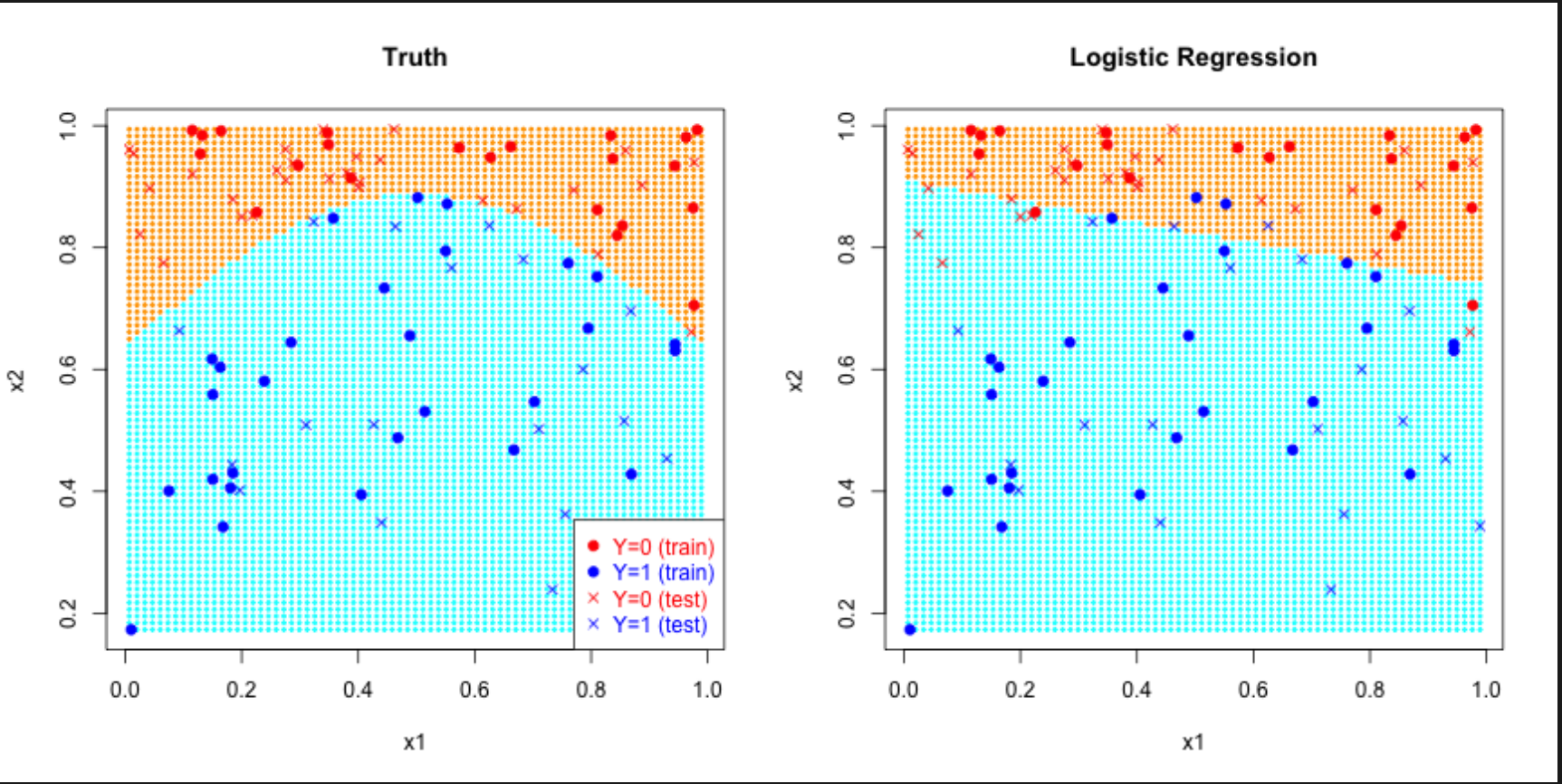
$$\text{logit}(p(y_i)) = \ln\left(\frac{p(y_i)}{1 - p(y_i)}\right) = \vec{x}_i \cdot \beta + e_i$$

- The model then assumes $y_i \sim \text{Bern}(p(y_i))$. The prediction is the **log-odds** ratio, with values > 0 predicting a 1 and values < 0 predicting a 0.

Logistic Regression fitting

- Logistic regression is an example of a **generalised linear model** or **GLM**.
- In general these cannot be directly solved with Linear Algebra. Options include:
- **Maximum likelihood** estimation:
  - A numerical procedure can be used to maximise the likelihood in terms of the parameters β, and σ the variance of e.
- Iteratively Reweighted **least squares** (IRLS):
  - The non-linearity can be adopted into weights, and a linear algebra solution reached.
  - Then the weights are updated, and the procedure iterated.
- Co-estimation tends to be relatively computationally costly (higher dimensional space) but to have better estimation properties.
- In both cases we look for sub-problems that can be efficiently solved.

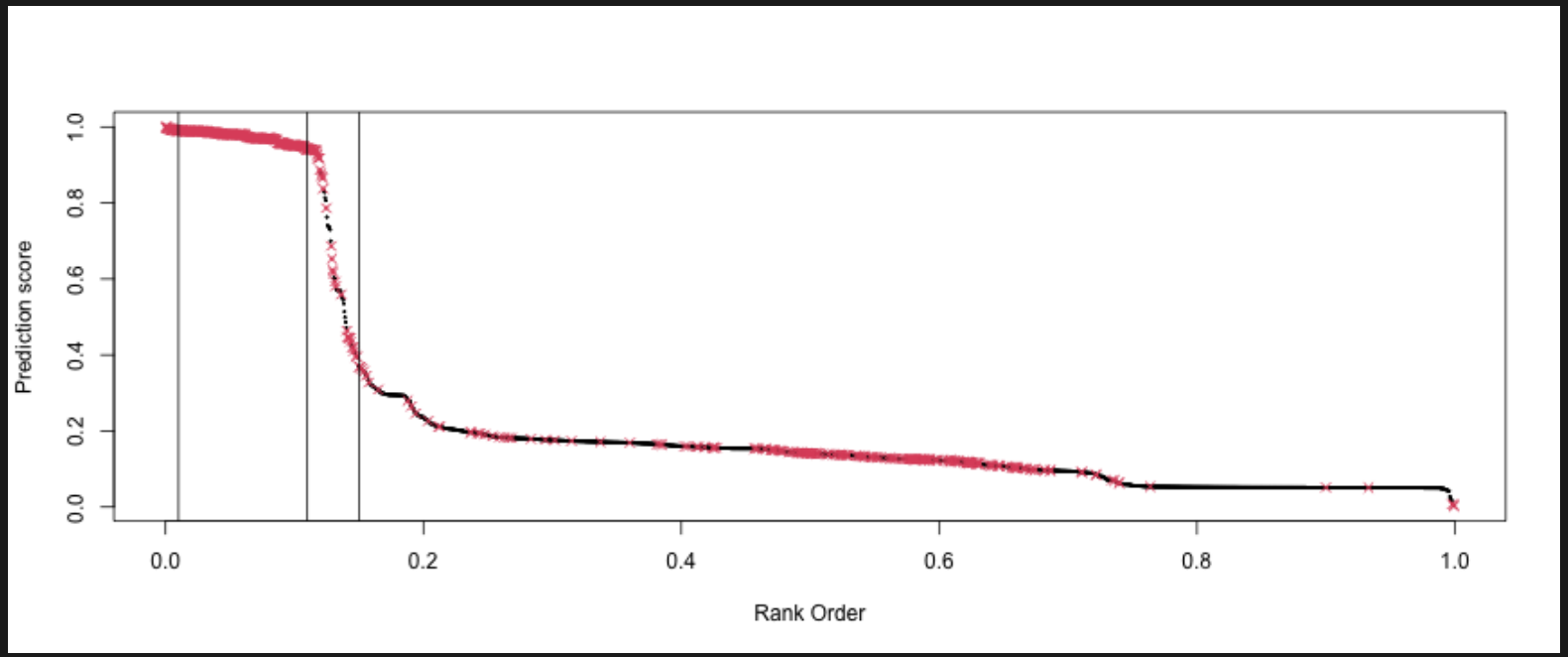
Logistic Regression example



Classification Performance

- We can always compute **training** and **test** dataset accuracy.
- However, we should only ever compare performance on **test** data, to prevent over-fitting.
- Classifiers are understood through their **Confusion Matrix**, that is a comparison between:
  - Ground truth class, and
  - Predicted classes.
- For binary classes, we summarise using (true/false)(positive/negative) outcomes.
- Binary classification is particularly convenient as most classifiers can provide **scores** rather than **class predictions**.
  - Scores are **ordered**. So we can choose a threshold to control the total proportion of **positive predictions**.
  - This provides a **relationship** between **Positive Claims** and **True Positives**.

Classification Performance



.	$Y = 1$	$Y = 0$	Condition
$\hat{Y} = 1$	TP	FP	Prediction positive
$\hat{Y} = 0$	FN	TN	Prediction negative
Claim	Truth positive	Truth Negative	.

Classification Performance Representations

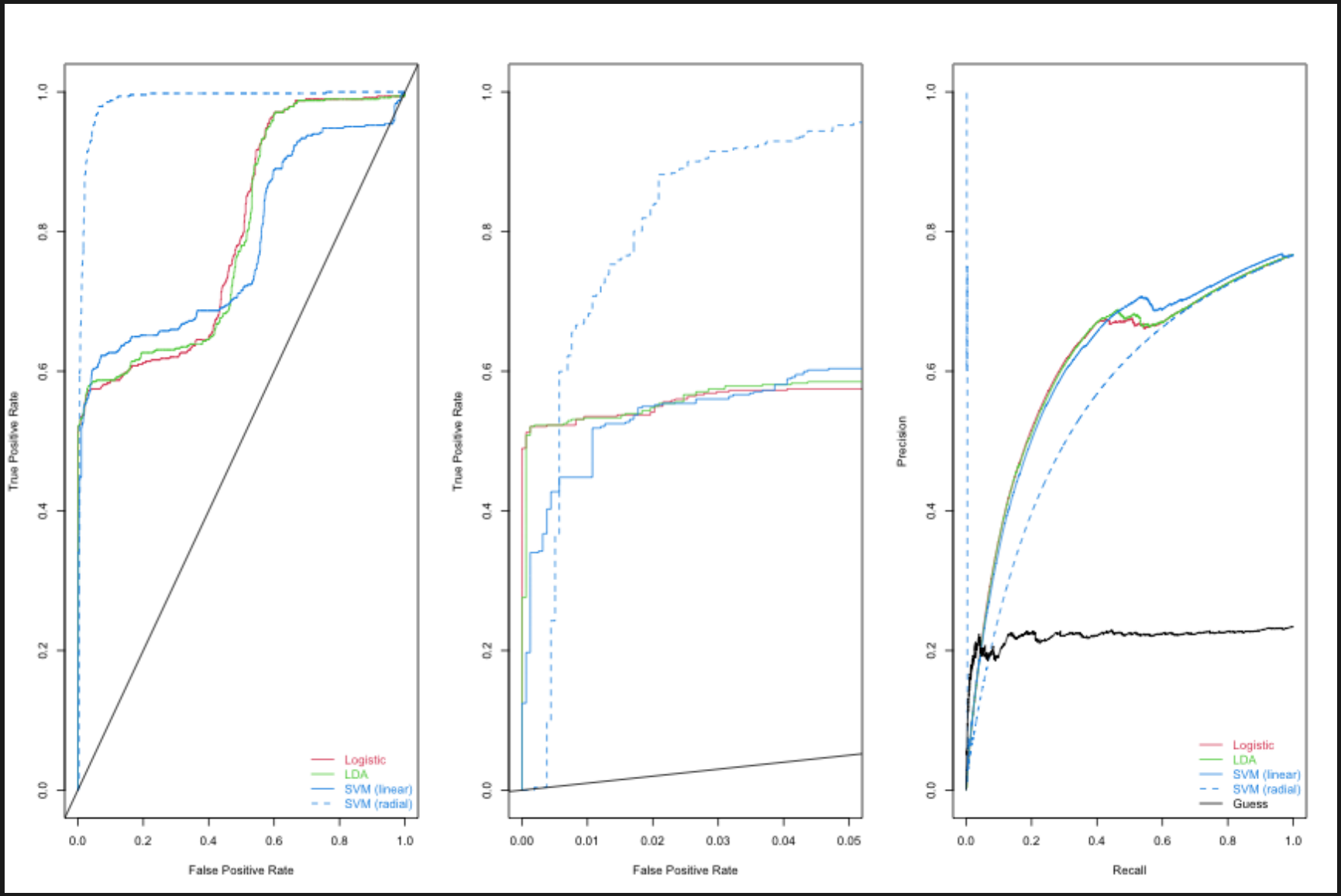
- There are many ways to represent performance
- The **Receiver-Operator-Curve (ROC)** is the most popular, as it holds regardless of the true distribution of the data.
  - X-axis: False Positive Rate (FPR) $= P(\hat{Y} = 1|Y = 0)$
  - Y-axis: True Positive Rate (TPR) $= P(\hat{Y} = 1|Y = 1)$
  - The **Area Under the Curve (AUC)** is a measure of Accuracy (0.5=guessing, 1=perfect).
  - We need to care about the region of the ROC curve that matters.
- The **Precision-Recall curve** is appropriate when we care specifically about positive cases:
  - X-axis: Precision $= P(Y = 1|\hat{Y} = 1)$
  - Y-axis: Recall=TPR $= P(\hat{Y} = 1|Y = 1)$

Some important properties

- Some nice things[1] can be said about ROC and PR curves:
- Dominance:
  - If one curve dominates (is always above) another in ROC, it dominates in PR
  - and vice-versa
- ROC curves can be linearly interpolated
  - This is "flipping a coin" to access classifiers in-between
- PR curves have a slightly more complex relationship but the same principle can be applied
- Integrating both scores leads to performance metric that can be optimized

[1] Davis and Goadrich, "The Relationship Between Precision-Recall and ROC Curves", ICML 2006.

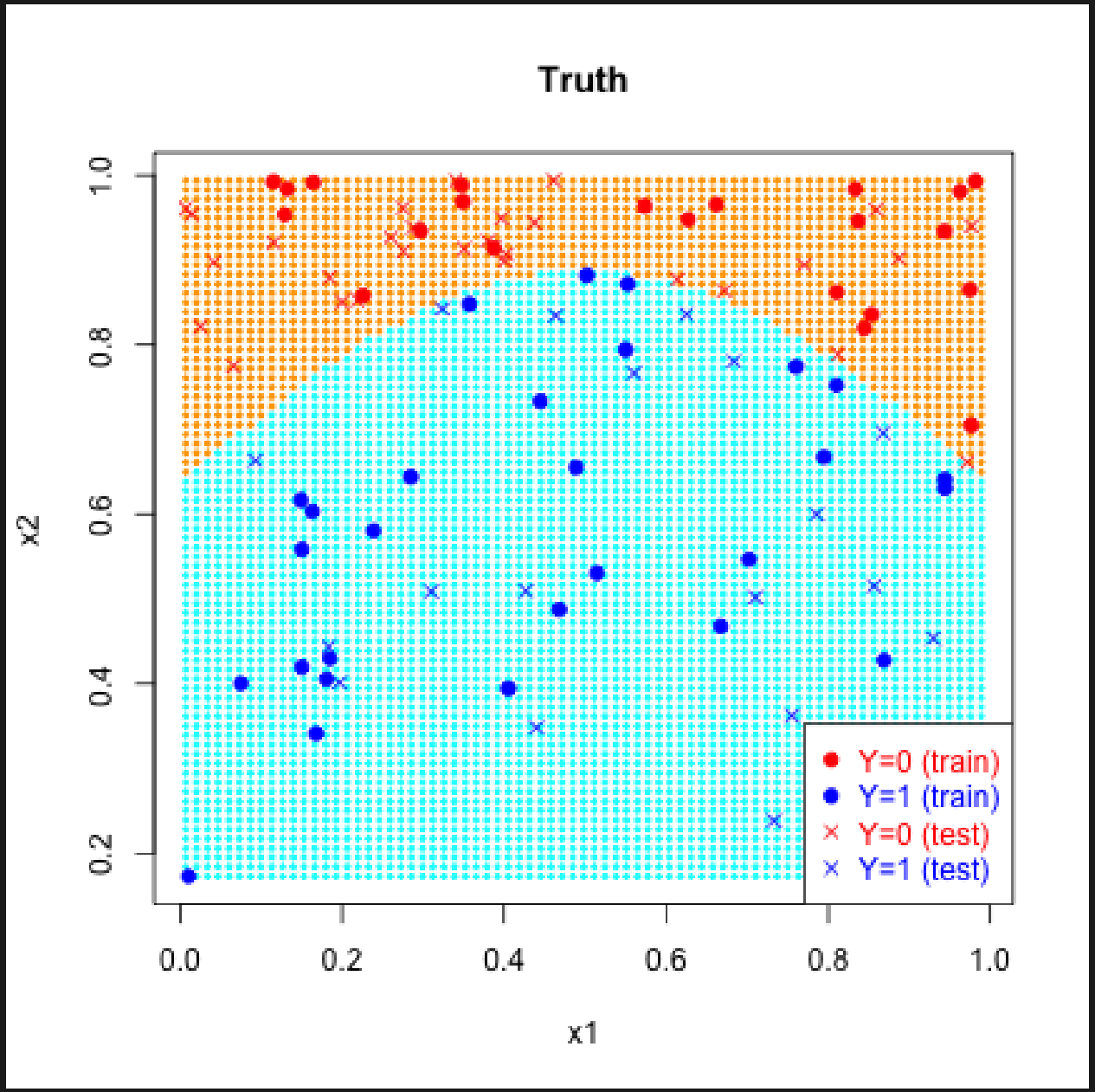
ROC/PR Curve Example



Metrics for Classification

- Accuracy (Proportion of samples classified correctly) is a terrible metric if classes are unequal
- TPR at a given FPR is more flexible
- AUC characterises the whole ROC curve
- Area Under Precision-Recall Curve (AUPRC?) is also a thing people advocate for
- None are "right", we have to define the inference task
- Any of these and more are often optimized
  - If we optimise a parameter or perform model comparison based on test data, we need additional test data to test the meta-algorithm!

Classification

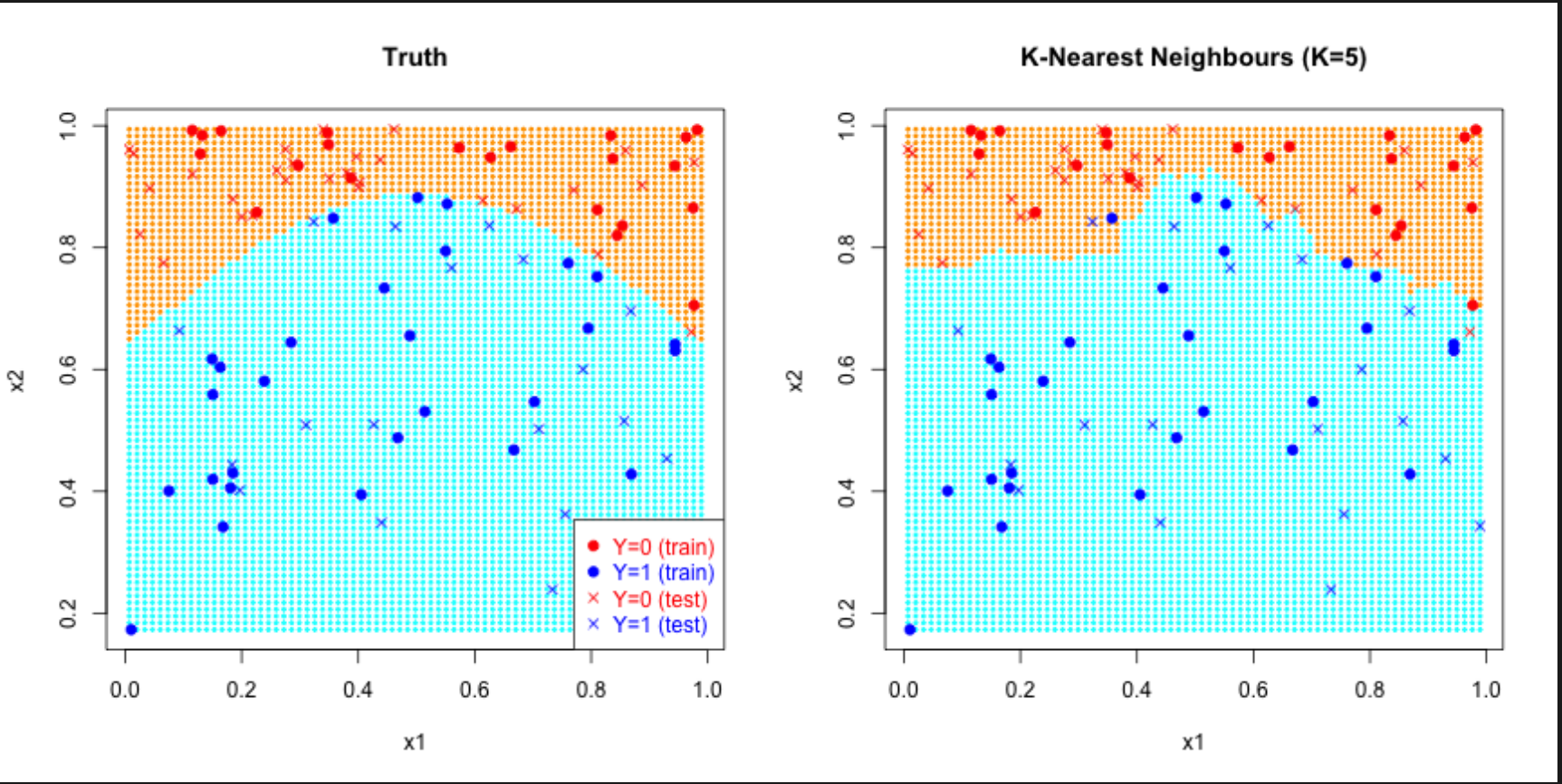


K-Nearest Neighbour classification

- In Block 4, we introduced K-NN for density estimation.
  - We defined some choices of distance function
  - We obtained the K nearest neighbours of points in R
- Armed with those neighbours, a classifier can be implemented by using **majority vote** of the labels of all k neighbours.
- A naive implementation scales poorly with N, but an approximate lookup can control complexity.
- See also: Condensed nearest neighbor[2] approaches to reduce the amount of data required at the classification stage.

[2] Hart P, The Condensed Nearest Neighbor Rule. IEEE Transactions on Information Theory 18 (1968) 515-516. doi: 10.1109/TIT.1968.1054155

K-Nearest Neighbour example



Linear Discriminant Analysis

- Developed in **1936 by R. A. Fisher**[3] and extended to the current multi-class form in 1948[4].
- The goal is to **project** a high dimensional space into K dimensions, **maintaining** (linear) classification ability.
- Prediction benefit comes only from reducing overfitting
- Strong **relationship with PCA**, often used in tandem (PCA then LDA)
- Assumes that each class k has a different mean μ_k and a shared covariance matrix Σ
- Kernel Discriminant Analysis exists[5]

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[3] Fisher R, "The Use of Multiple Measurements in Taxonomic Problems" (1936) Annals of eugenics (!), now "Annals of Human Genetics"

[4] Rao C, "Multiple Discriminant Analysis" (1948) JRSSB

[5] Mika, S et al "Fisher discriminant analysis with kernels" (1999) NIPS IX: 41-48

LDA algorithm

1. Compute the mean location μ_k for each class k and the overall mean μ, as well as the assignment sets D_k.
2. Compute the **within-class scatter matrix** S_W:
   $S_W = \sum_{k=1}^{K} S_k$ where

$$S_k = \sum_{i \in D_k} (\vec{x} - \vec{\mu}_k) (\vec{x} - \vec{\mu}_k)^T$$

3. Compute the **between-class scatter matrix** S_B:

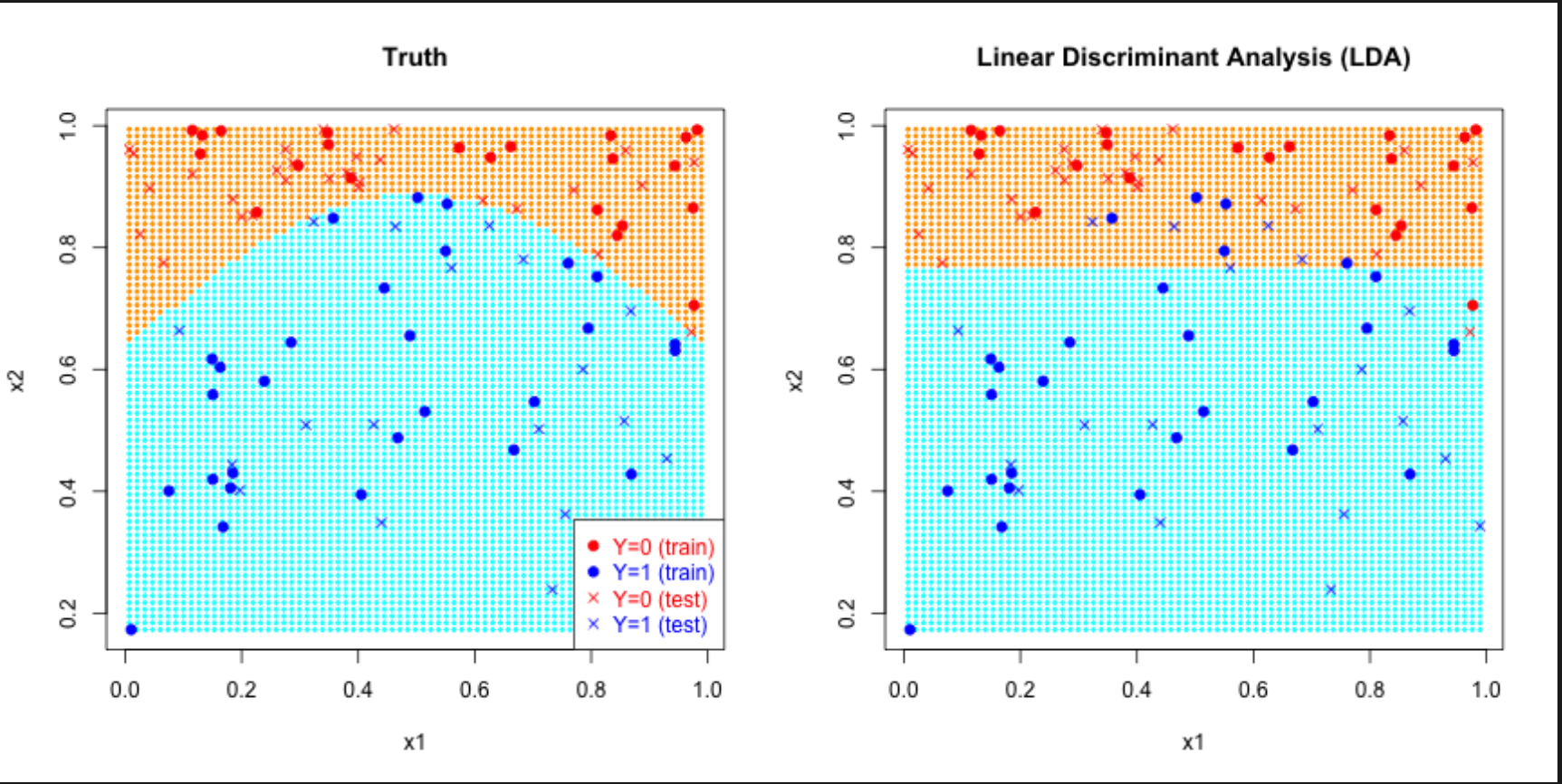
$$S_B = \sum_{k=1}^{K} n_i (\vec{\mu}_k - \vec{\mu}) (\vec{\mu}_k - \vec{\mu})^T$$

4. Solve for the **eigenvalues** λ_k and **eigenvectors** v_k of $S_W^{-1} S_B$
5. **Choose a dimension** threshold K^*, either using the same methods as for PCA, or cross-validation
6. **Predict** using μ_k ...

LDA prediction

- Class prediction can use any information in the LDA data summary. Options include:
  - Nearest cluster
  - **Likelihood**: $\Pr(\vec{x}|y_k = c) = \text{Normal}\,(\mu_k, \Sigma)$
  - **Posterior**: $\Pr(y_k = c|\vec{x}) \propto \Pr(\vec{x}|y_k = c)p(y_k = c)$; i.e. reweight classes according to their frequency

LDA example


Truth
Linear Discriminant Analysis (LDA)
x1
x2
0.0
0.2
0.4
0.6
0.8
1.0
Y=0 (train)
Y=1 (train)
Y=0 (test)
Y=1 (test)

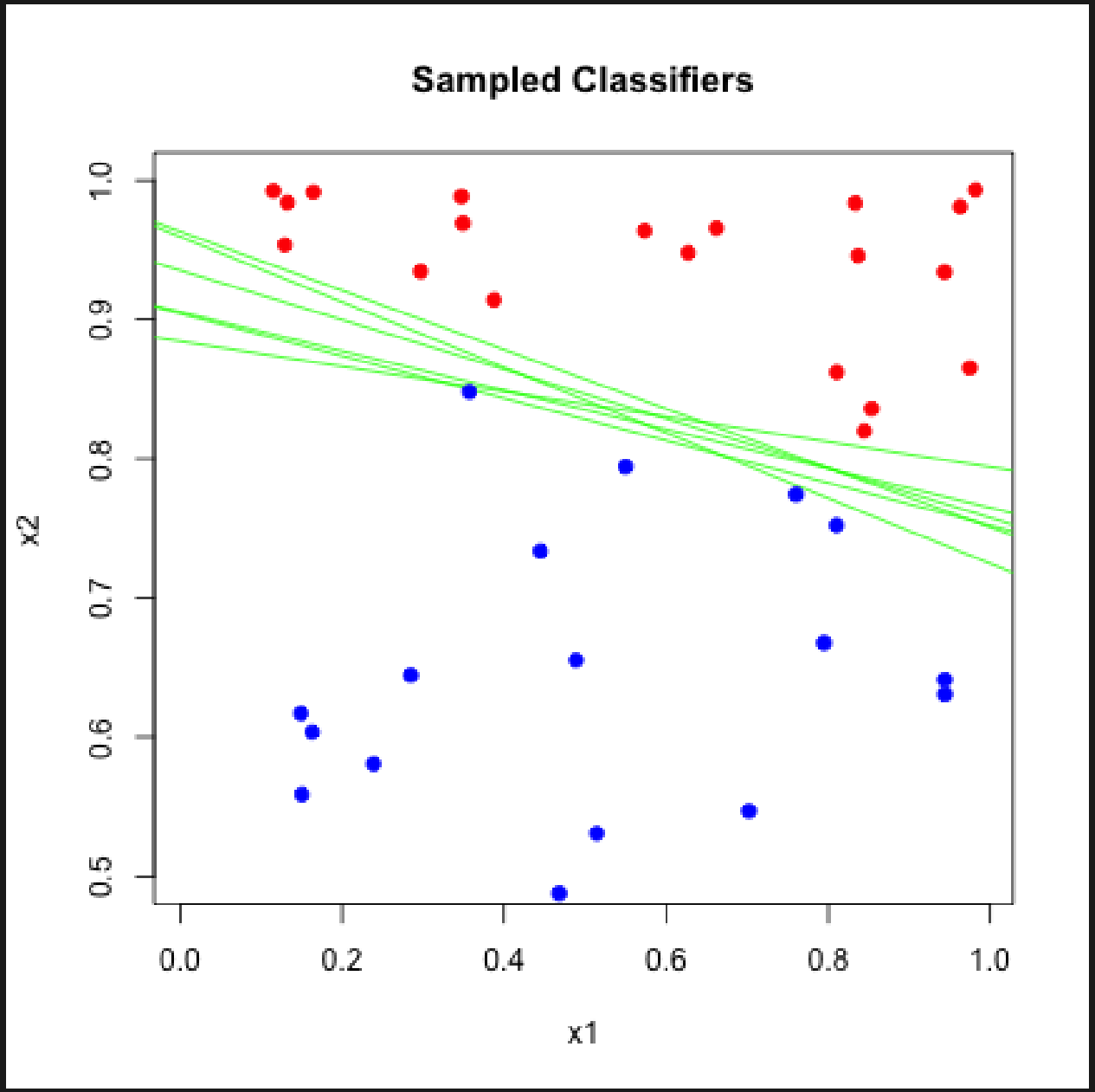
Towards Support Vector Machines

- LDA uses **all the points** for classification, which makes it slow
- It is also **linear**
- (It could be made non-linear by mapping the data to high dimensions, but this is often infeasible)
- Moving towards SVM, we:
  - Can exploit the **kernel-trick** to make a non-linear decision boundary without explicit mapping
  - Switch focus from group **means** to making the largest group **separation**
  - If we only want to **discriminate classes**, we can only use a subset of the data, the **support vectors**, for the decision
- This makes the method:
  - robust to distributional assumptions
  - non-generative

Support Vector Machine overview

- Find the **maximum margin hyperplane** separating the classes **closest** points
- Allow soft margins: misclassified points are down-weighted
- Nonlinearity: express distances as **inner products**, allowing non-linearities via the Kernel trick
- Algorithm: finding the hyperplane is a "quadratic optimisation problem".

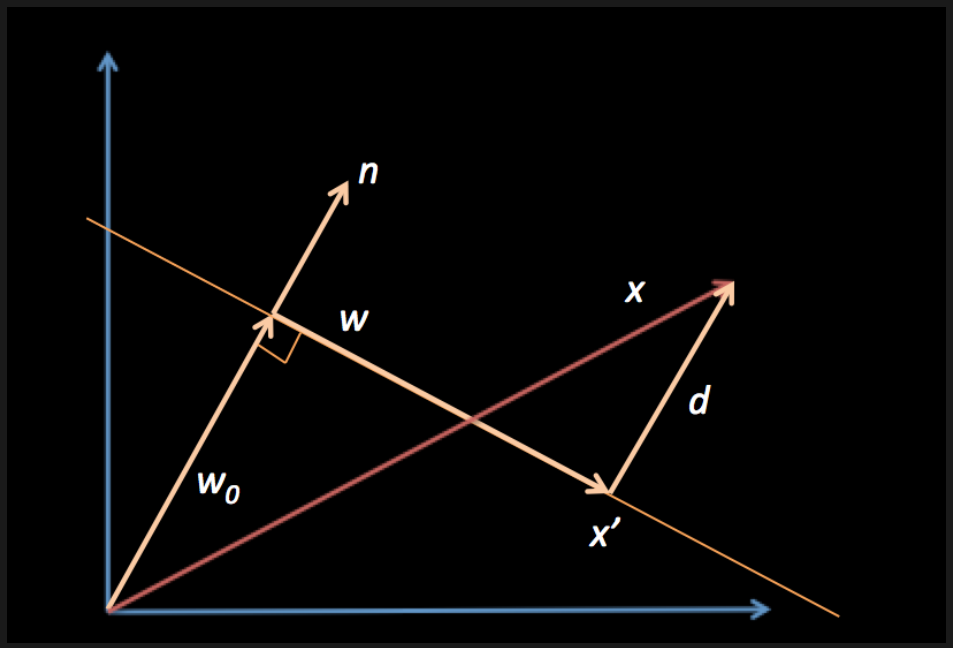
SVM illustration: solution space



Planar geometry

- The data are $\vec{x} \in D$ containing N examples
- The labels are $y_i \in (-1, 1)$
- A **hyperplane** is defined via:
  - $\vec{w}$, the coordinates of the plane
  - $\vec{w}_0$, a point on the plane chosen such that $\vec{w}_0$ is perpendicular to $\vec{w}$:

$$\vec{w} \cdot (\vec{x} - \vec{w}_0) = \vec{w} \cdot \vec{x} + b = 0$$



SVM margins

- The **distance of a point to the line** is the residual after the point is projected onto the line:

$$d_{\vec{w}}(\vec{x}) = \vec{n} \cdot (\vec{x} - \vec{x}') = \frac{|\vec{w} \cdot \vec{x} + b|}{|\vec{w}|}$$

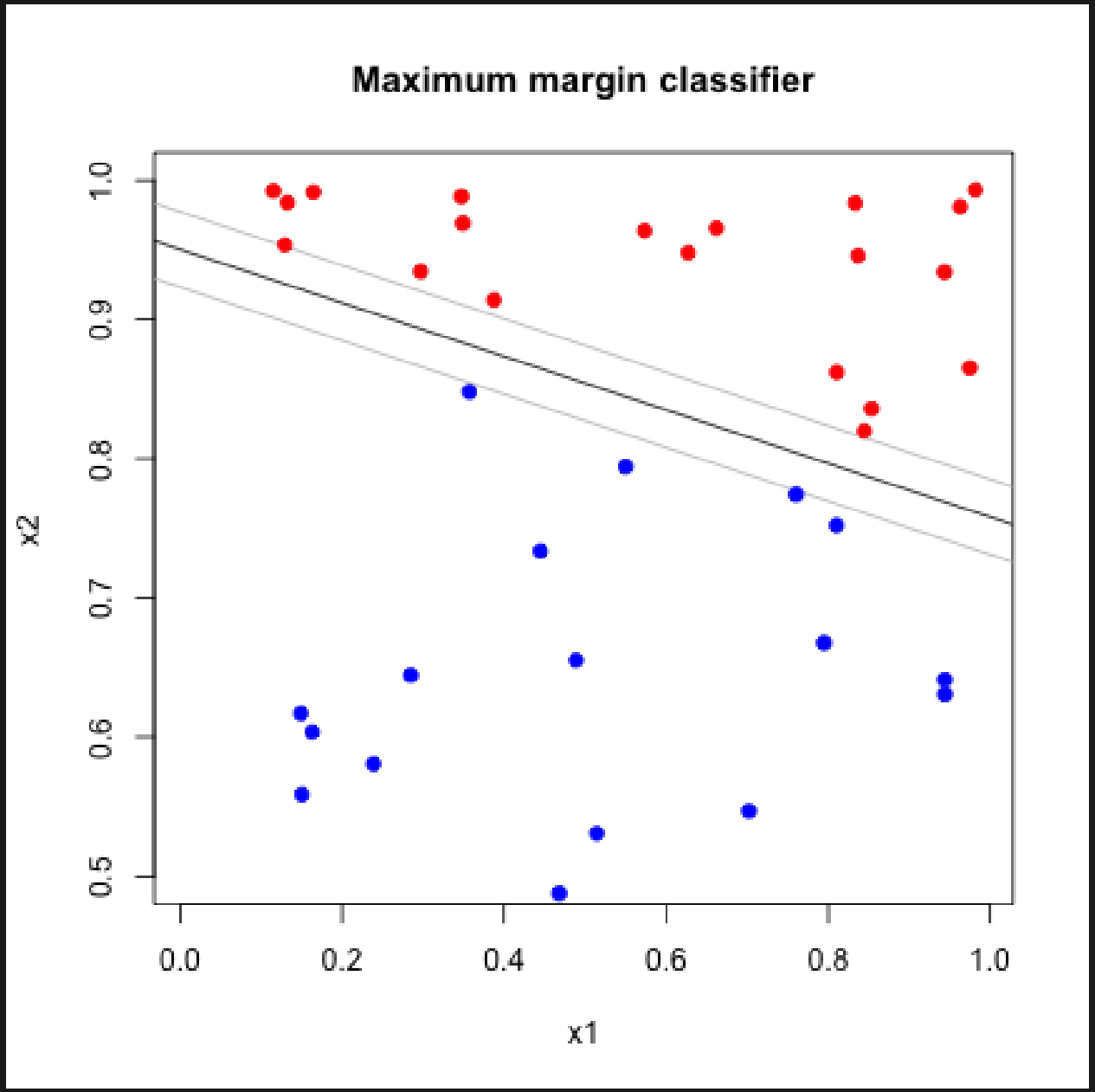
- For a given hyperplane, the **minimum margin** is

$$M_{\vec{w}} = \text{argmin}_{x \in D} d_{\vec{w}}(\vec{x})$$

- The **maximum margin hyperplane** is therefore:

$$\text{argmax}_{\vec{w}} \text{argmin}_{x \in D} d_{\vec{w}}(\vec{x})$$

SVM illustration: SVM solution

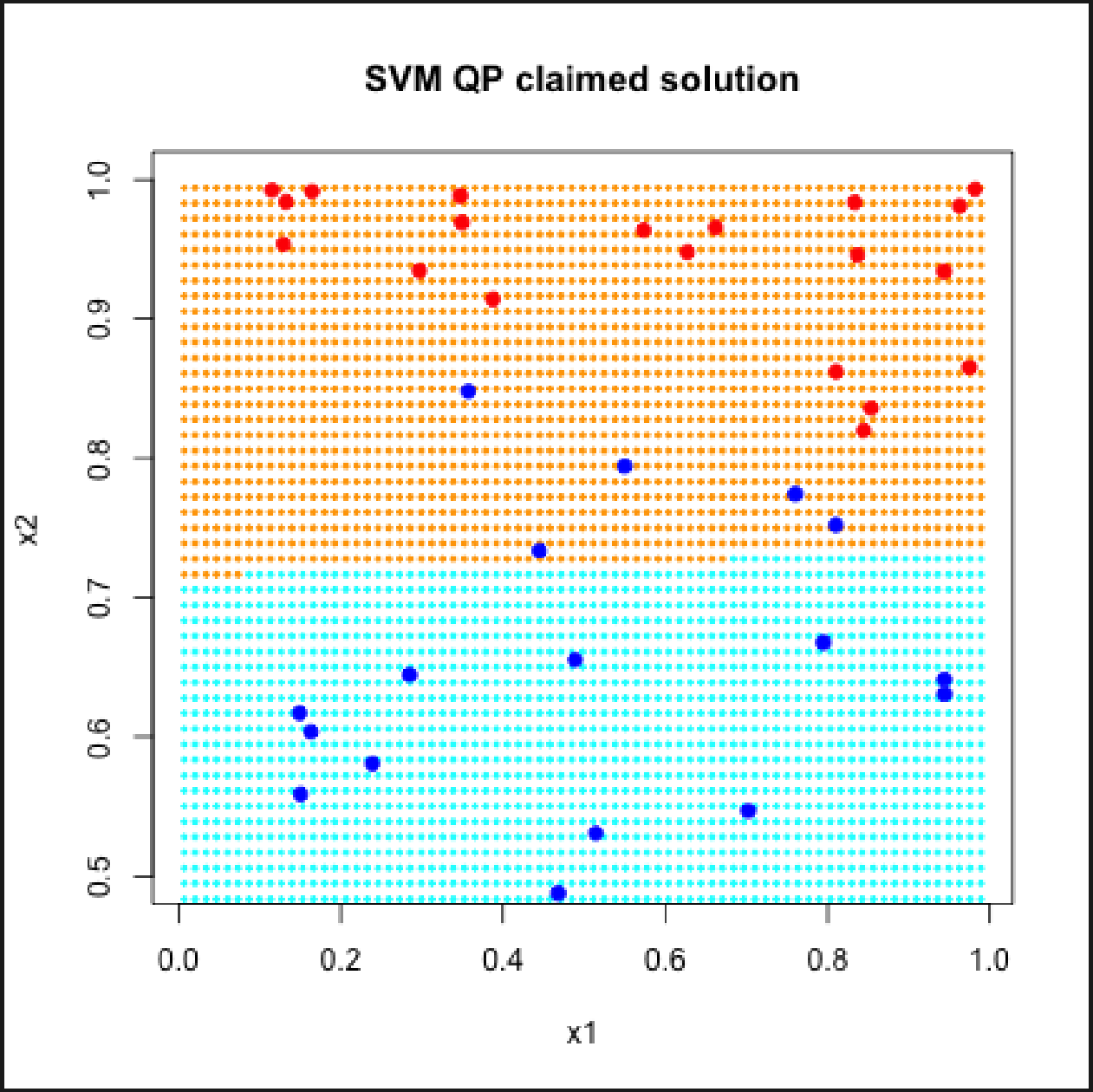


Computing the margins

- This is a classic **Quadratic Programming** problem[6]
- Broadly:
  - quadratic penalty: distance to the plane $\propto$ squared norm of the hyperplane vector $\frac{1}{2}|\vec{w}|^2$
  - linear inequalities: none of the data are closer than $M_{\vec{w}}$. So $\forall i : y_i(\vec{w} \cdot \vec{x} + b) \geq 1$
- and pass these to a standard QP solver
- A computational trick: only evaluate the points on the margins

[6] For this course, you need to know what QP can do for you. You don't need to know how it works.

SVM problem



Imperfect classification with SVM

- To account for data the **wrong side of the margins**, the penalty is changed to:

$$\frac{1}{2}\left|\vec{w}\right|^2 + C\sum_{i=1}^{N}\epsilon_i$$

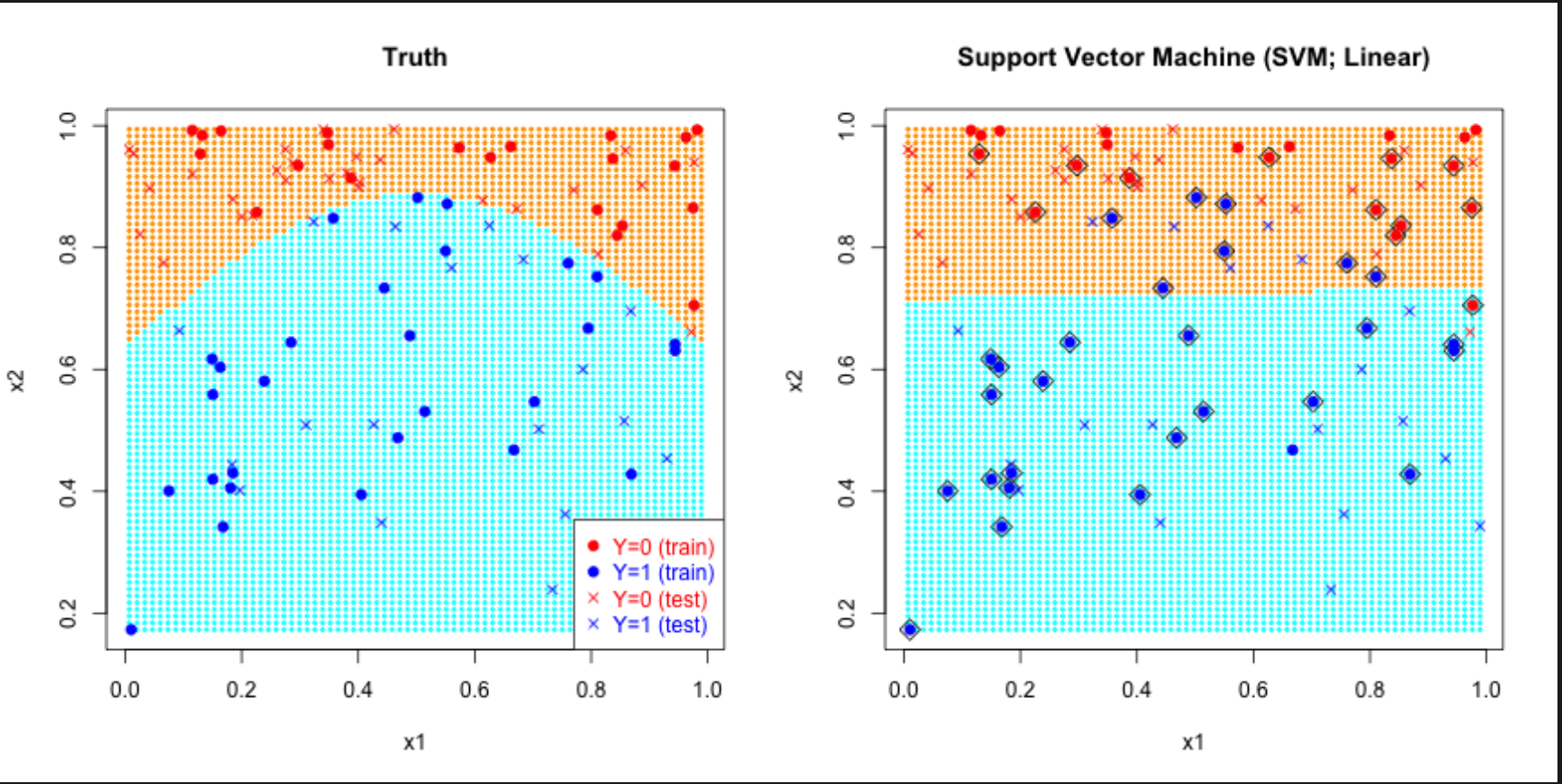
- where ϵ_i is the "distance" needed to move the point to the correct decision boundary, i.e.

$$\vec{w}\cdot\vec{x}_i + b \geq 1 - \epsilon_i \qquad \text{if :} \qquad y_i = 1 \quad (1)$$

$$\vec{w}\cdot\vec{x}_i + b \leq -1 + \epsilon_i \qquad \text{if :} \qquad y_i = -1 \quad (2)$$

- and $\epsilon_i = 0$ if already inside it, so also requiring the constraint $\epsilon_i \geq 0$

SVM example


Truth
Support Vector Machine (SVM; Linear)
x1
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Y=0 (train)
Y=1 (train)
Y=0 (test)
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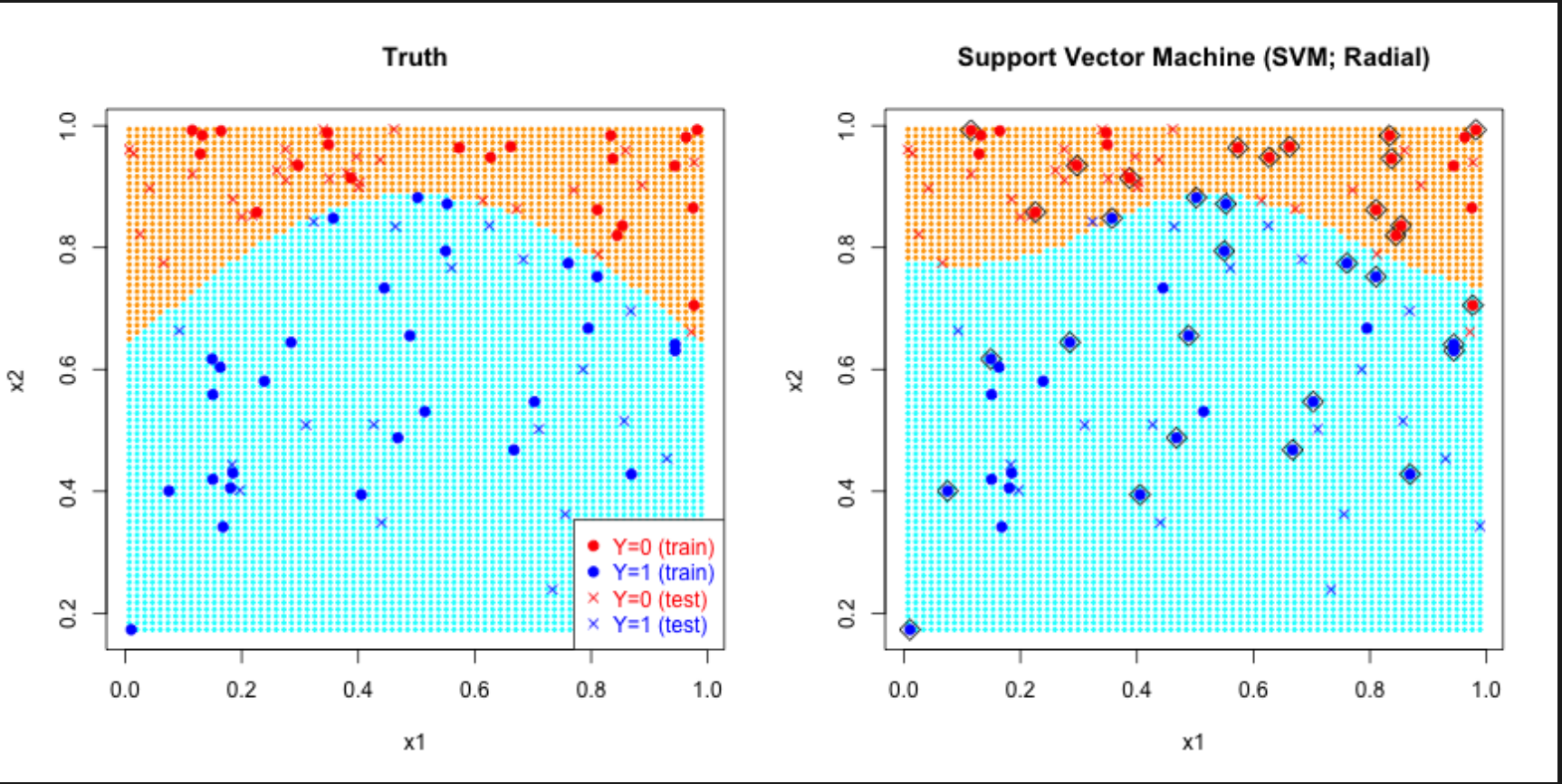
kernel SVM example



Wrapup

- **Logistic regression** is the go-to straw man classifier in machine learning:
  - It is easy to implement
  - It is a natural predictive model
  - It does reasonably well in many settings
- **k-NN** is the interpolation method to beat
- **Linear Discriminant Analysis** is also widely used:
  - It is easy to bolt onto PCA
  - Clusters are more **interpretable** than logistic regression
- **SVMs** remain an important competitor at the bleeding edge:
  - A hyperplane is a natural **discriminatory model**
  - Feature engineering can allow complex **non-linear** models
  - Low-complexity classifier once training is performed
- **Neighbourhoods** are always competitive, but are costly at test time

Reflection

- Why is LDA used with PCA, and not instead-of?
- How would you imagine an approximate lookup for k-NN would work?
- How sparse should the SVM solution be? In what sense is SVM efficient? When would it be cutting edge?
- By the end of the course, you should:
  - Be able to navigate the many approaches to classification
  - Understand and be able to explain the high level function of:
  - Logistic Regression, Nearest Neighbour classification, LDA, SVMs

Signposting:

- In this Block's workshop we'll experiment with these and other classifiers on cyber data, as well as introducing **boosting**.
- In the following Block we'll introduce Random Forests, as well as boosted decision and regression trees. Naive Bayes comes in Block 7 with other Bayesian Methods.
-
- **References** for classification basics:
  - Stack Exchange Discussion of ROC vs PR curves.
  - Davis and Goadrich, "The Relationship Between Precision-Recall and ROC Curves", ICML 2006.
  - Rob Schapire's ML Classification features a Batman Example...
  - Chapter 4 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
- k-Nearest Neighbours:
  - Chapter 13.3 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
- Linear Discriminant Analysis:
  - Sebastian Raschka's PCA vs LDA article with Python Examples