Lecture 5: Linear Models for Classification

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SoE, Westlake University

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Reading materials & Reference

Reading materials:

- Chapter 3, Stanford CS 229 Lecture Notes, https://cs229.stanford.edu/notes2022fall/main_notes.pdf
- Lecture 4, Stanford CS 231n, http://cs231n.stanford.edu/schedule.html

Reference:

- EPFL, CS-433 Machine Learning, https://github.com/epfml/ML_course

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How do we trade-off the under-fitting and over-fitting?

Probabilistic setup

Data model:

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- S denotes the input (dataset).

True Error, Empirical Error, and Training Error

- **True Error** (the **expected error** over all samples chosen according to $\mathcal{D}$):

$$\mathcal{L}_{\mathcal{D}}(f) = \mathbb{E}_{\mathcal{D}}\left[\ell(y, f(\mathbf{x}))\right] . \tag{3}$$

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The reason that $L_S(f_S)$ might not be close $L_{\mathcal{D}}(f_S)$ is of course over-fitting.

Problem: validating the model on the same data subset we trained it on!

Splitting the data and Test Error

- **Fix:** Split the data into a *training* set S_{train} and a *test* set S_{test} (a.k.a. *validation* set):

$$S = S_{\text{train}} \bigcup S_{\text{test}} \tag{6}$$

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$$L_{S_{\text{test}}}(f_{S_{\text{train}}}) = \frac{1}{|S_{\text{test}}|} \sum_{(y_n, \mathbf{x}_n) \in S_{\text{test}}} \ell\left(y_n, f_{S_{\text{train}}}(\mathbf{x}_n)\right). \tag{7}$$

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- Issues: we have fewer data both for the learning and validation tasks (trade-off)

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Generalization gap: How far is the test from the true error?

- **True Error:**

$$L_{\mathcal{D}}(f) = \mathbb{E}_{(y,\mathbf{x})\sim\mathcal{D}}\left[\ell\left(y, f(\mathbf{x})\right)\right]. \tag{8}$$

- **Test/Empirical Error:**

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The variation of the $\left|L_{\mathcal{D}}(f) - L_{S_{\text{test}}}(f)\right|$ matters.

Theorem 1

Given a model f and a test set $S_{test} \sim \mathcal{D}$ i.i.d. (not used to learn f) and a loss $\ell(\cdot,\cdot) \in [a,b]$:

$$\Pr\left[|L_{\mathcal{D}}(f) - L_{S_{test}}(f)| \geq \sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2\,|S_{test}|}}\right] \leq \delta \tag{12}$$

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Given a predictor f and a dataset S, we can control the expected risk:

$$\Pr\left[\underbrace{L_{\mathcal{D}}(f)}_{\text{not computable}} \geq \underbrace{L_{S_{\text{test}}}(f)}_{\text{computable}} + \underbrace{\sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2\,|S_{\text{test}}|}}}_{\text{deviation}}\right] \leq \delta\,. \tag{13}$$

How far is each of the K test errors $L_{S_{\text{test}}}(f_k)$ from the true $L_{\mathcal{D}}(f_k)$?

Theorem 2

We can bound the maximum deviation for all K candidates, by

$$\Pr\left[\max_k |L_{\mathcal{D}}(f_k) - L_{S_{test}}(f_k)| \geq \sqrt{\frac{(b-a)^2 \ln(2\boxed{K}/\delta)}{2|S_{test}|}}\right] \leq \delta \tag{14}$$

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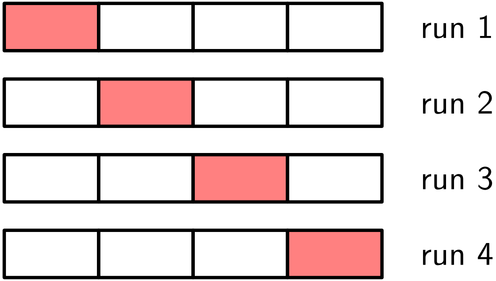
$\Rightarrow$ So we can test many different models without incurring a large penalty.

Issues: Splitting the data once into two parts (one for training and one for testing) is not the most efficient way to use the data!

K-fold cross-validation:

1. Randomly partition the data into K groups
2. Train K times. Each time leave out exactly one of the K groups for testing and use the remaining $K-1$ groups for training.
3. Average the K results



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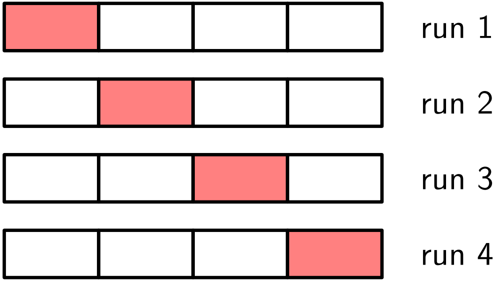

Benefits:

- We have used all data for training, and all data for testing, and used each data point the same number of times.

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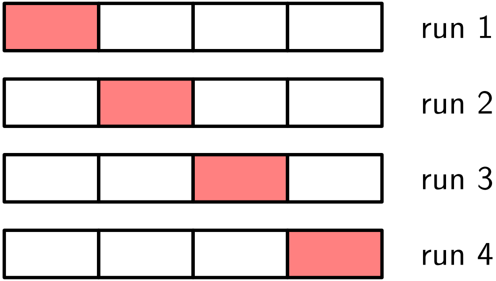

Benefits:

- We have used all data for training, and all data for testing, and used each data point the same number of times.
- Cross-validation returns an unbiased estimate of the generalization error and its variance.

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Bias-Variance Decomposition

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\begin{aligned}
\mathbb{E}_{S_{\text{train}} \in \mathcal{D}} \left[L(f_{S_{\text{train}}}) \right] = {} & \text{Var}_{\epsilon \sim \mathcal{D}_\epsilon} [\epsilon] && \text{(noise variance)} \\
& + \left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train}'}} \left[f_{S_{\text{train}'}}(\mathbf{x}_0) \right] \right)^2 && \text{(Bias)} \\
& + \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[\left(\mathbb{E}_{S_{\text{train}'}} \left[f_{S_{\text{train}'}}(\mathbf{x}_0) \right] - f_{S_{\text{train}}}(\mathbf{x}_0) \right)^2 \right], && \text{(Variance)}
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which always lower-bounds the true error.

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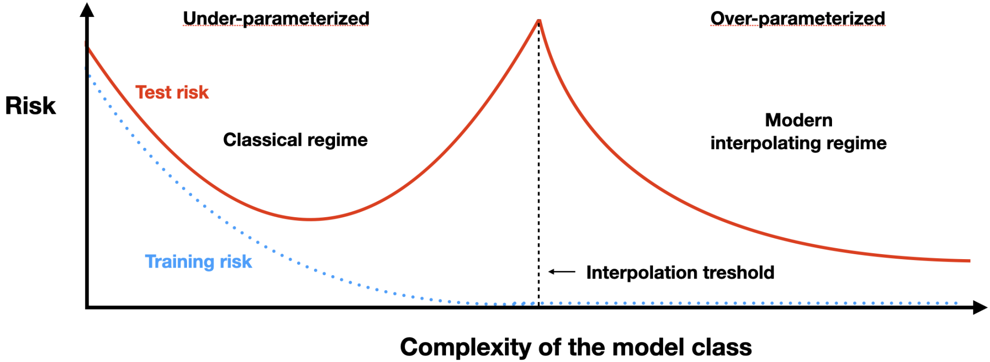
$\Rightarrow$ To minimize the true error, we need to select a method that **simultaneously achieves low bias and low variance**.

Double descent curve in Deep Learning



Last lecture:

- Generalization Gap and Model Selection
- Bias-Variance Decomposition

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This lecture:

- Logistic Regression
- Exponential Families and Generalized Linear Models

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Definition of classification

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How: relates input to a categorical variable

Classifier

A classifier $f : \mathcal{X} \to \mathcal{Y}$

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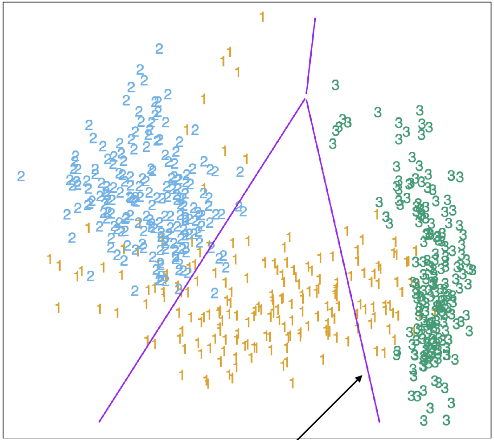

Linear Decision boundary

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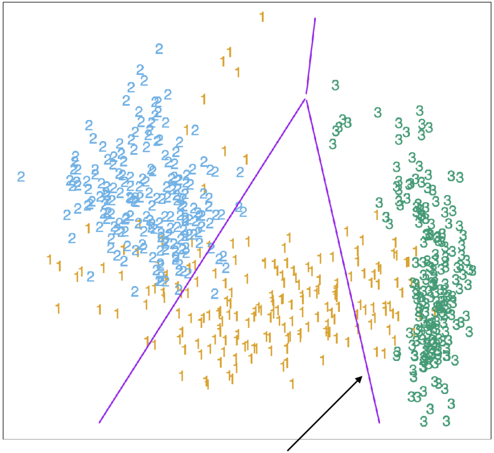

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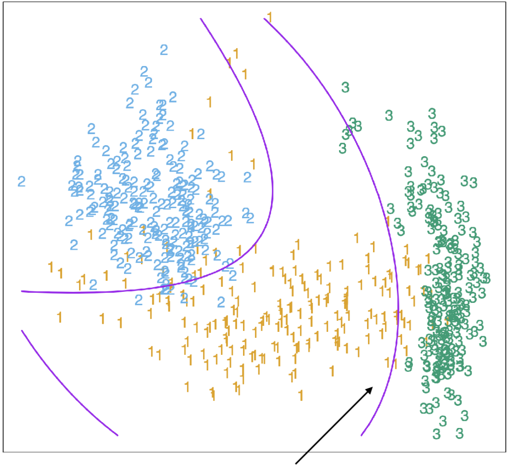

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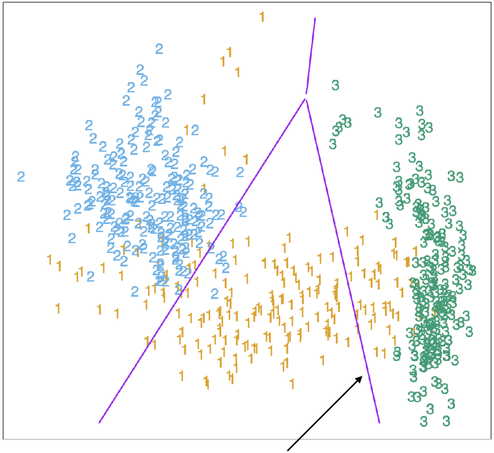

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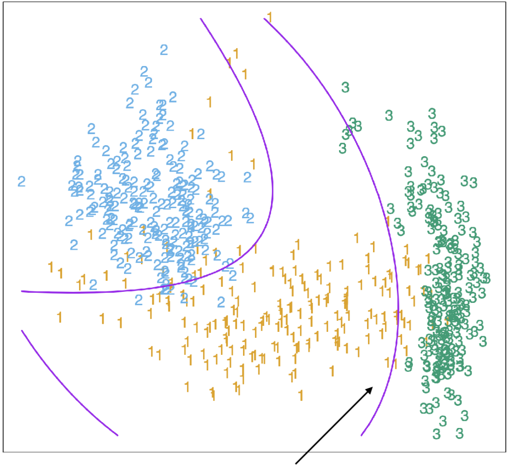

Nonlinear Decision boundary

Classification: a special case of regression?

Classification is a **regression problem** with discrete labels:

$$(\mathbf{x}, y) \in \mathcal{X} \times \{0, 1\} \subset \mathcal{X} \times \mathbb{R} \tag{15}$$

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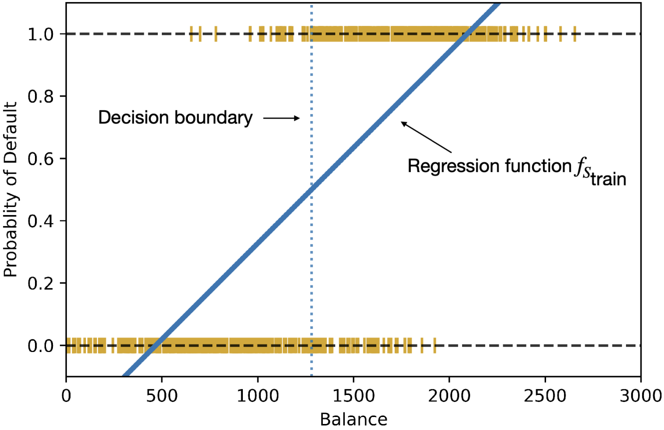
Could we use previously seen regression methods to solve it?

Is it a good idea to use some regression methods?



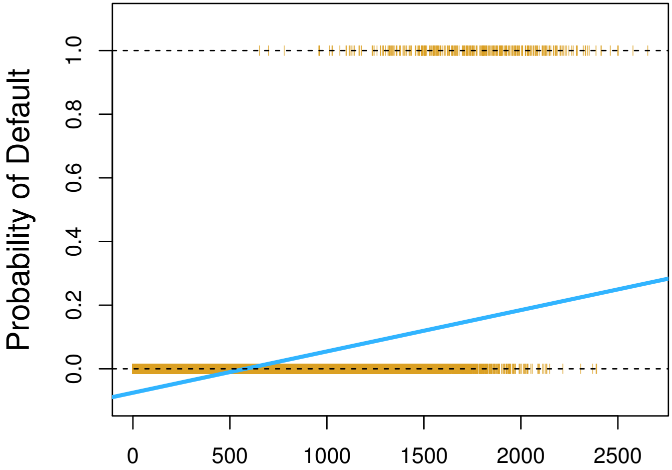
$y = 1$ **if "default"**

$y = 0$ **if "no default"**

We label the output as probability for sake of interpretation

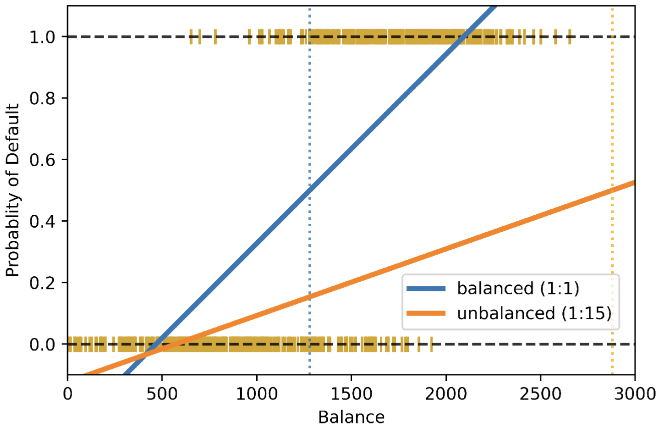
Classification is not just a special form of regression

- The predicted values are not probabilities (not in $[0, 1]$)



Classification is not just a special form of regression

- Sensitivity to unbalanced data



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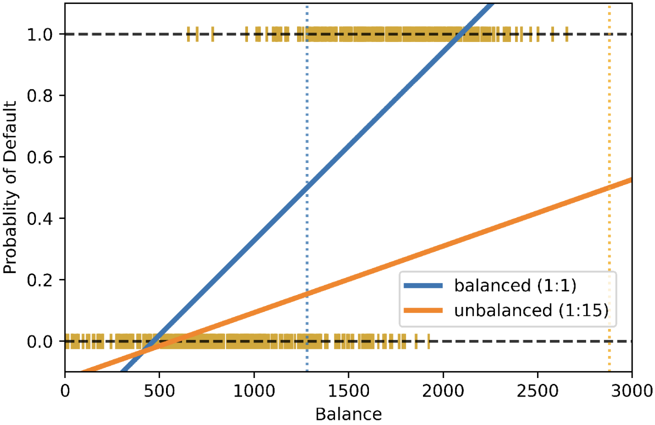

The position of the line depends crucially on how many points are in each class.

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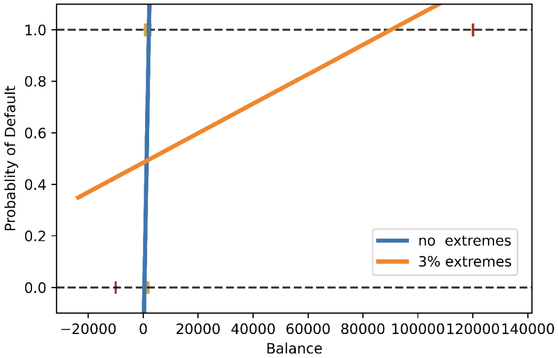
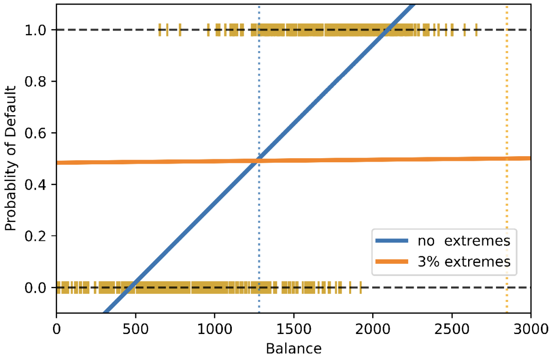
- Sensitivity to extreme values:





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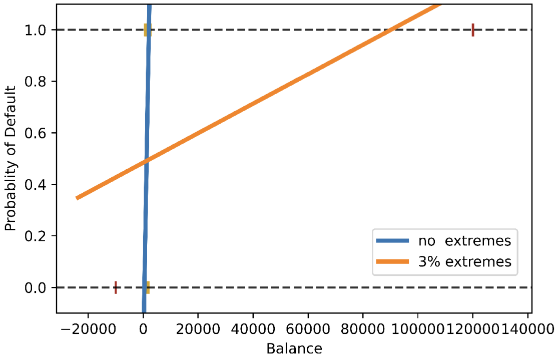

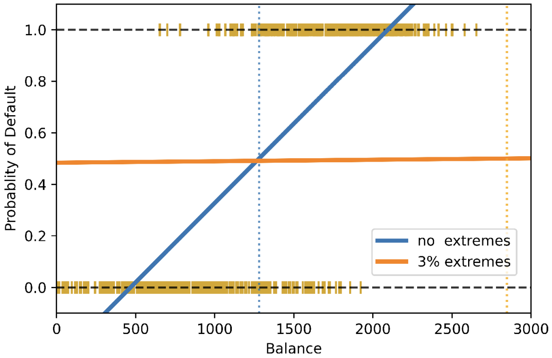

The position of the line depends crucially on where the points lie.

How to perform classification?

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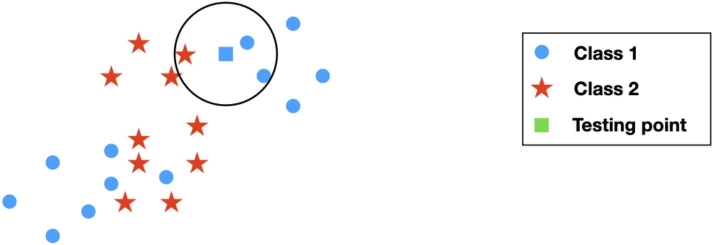
- Fundamental task of classification:

Divide the space into distinct decision regions

k-Nearest Neighbor

Assume that nearby points are likely to have similar labels



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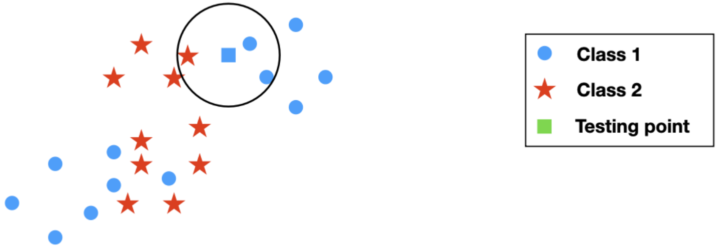

A new point $\mathbf{x}$ is classified based on the **majority vote of its k-nearest neighbors**.

k-Nearest Neighbor

Pros:

Cons:

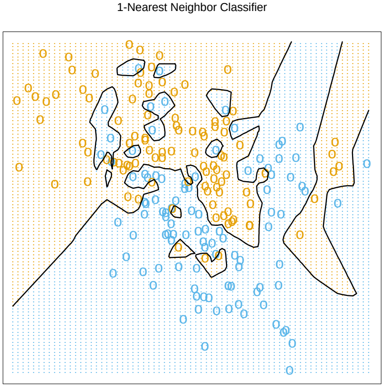

FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$)*, and then predicted by 1-nearest-neighbor classification.*

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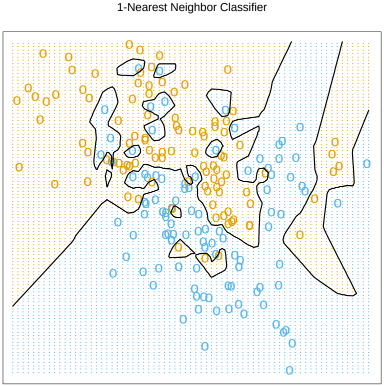

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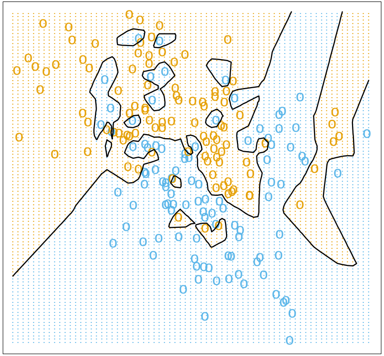

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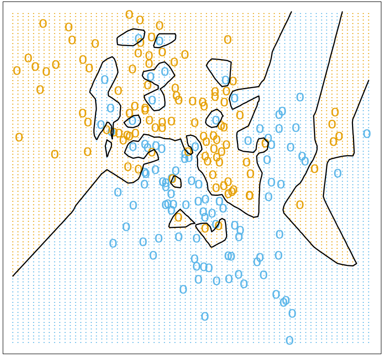

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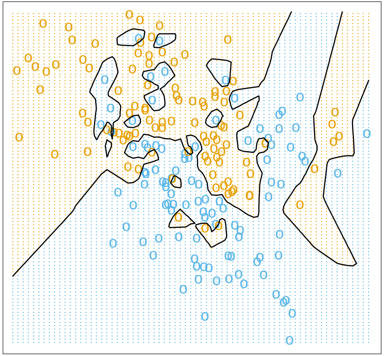

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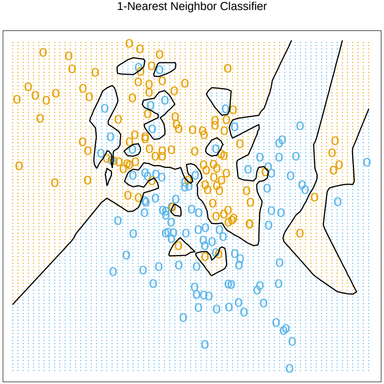

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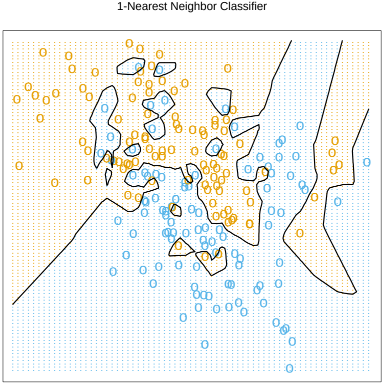

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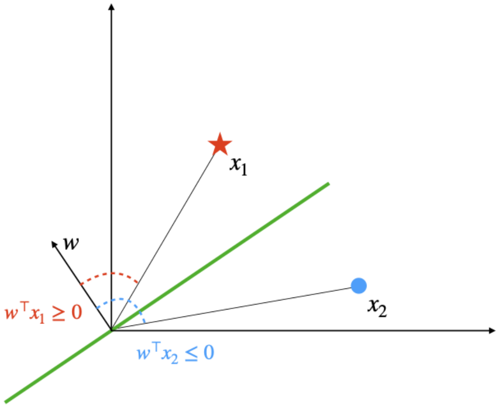

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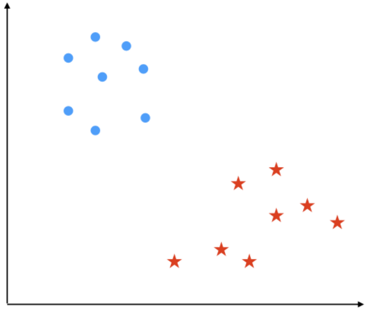

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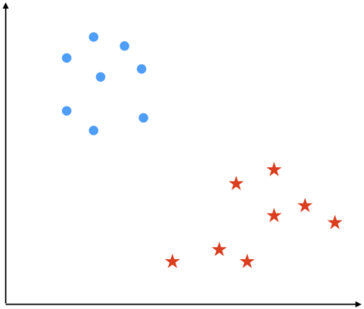

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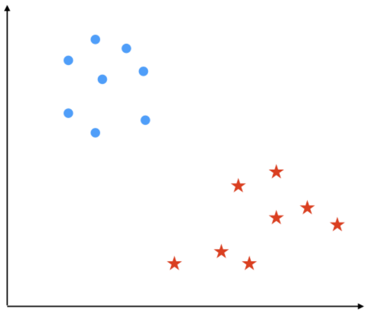

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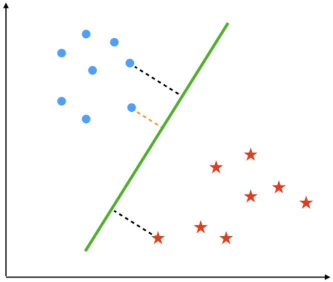
> Which separating hyperplane would you pick?

Margin

Key concept: The margin is the distance from the hyperplane to the closest point.



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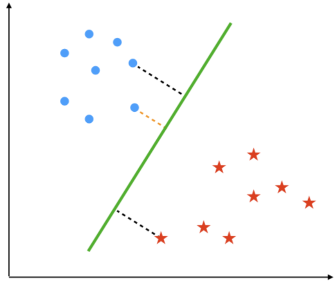
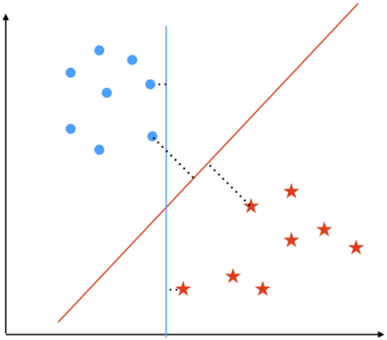


Take the one with the largest margin!

Max-margin separating hyperplane

Choose the hyperplane which maximizes the margin



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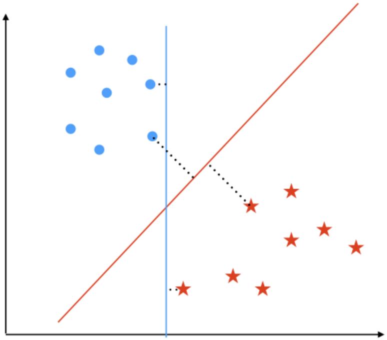

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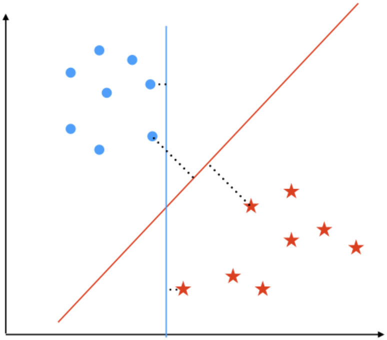

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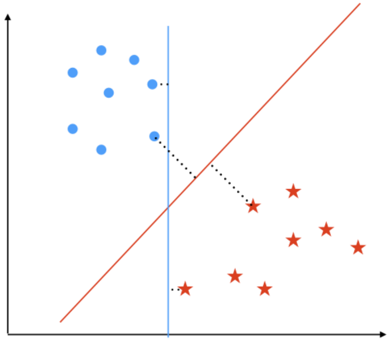
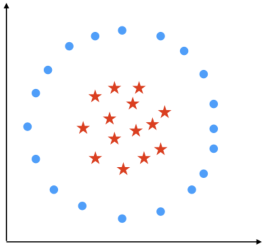


WHY? If we slightly change the training set, the number of misclassifications will stay low

⇒ It will lead us to support vector machine (SVM) and logistic regression!

Nonlinear classifier



Nonlinear classifier

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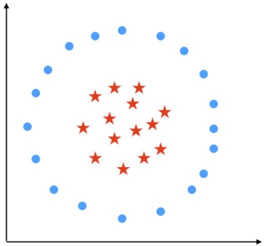

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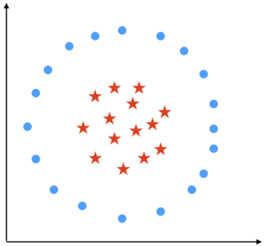

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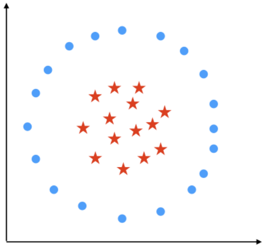

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- Goal: minimize $L_{\mathcal{D}}(f)$

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  But we can use the data to learn the distribution (by assuming the data distribution).

Proof of the Bayes classifier

Claim 1: $\forall \mathbf{x} \in \mathcal{X}, f(\mathbf{x}^\star) \in \arg\min_{y \in \mathcal{Y}} \Pr(Y \neq y | X = \mathbf{x}) \implies f^\star \in \arg\min_{f:\mathcal{X}\to\mathcal{Y}} L_{\mathcal{D}}(f)$

$$
\begin{aligned}
L_{\mathcal{D}}(f) = \mathbb{E}_{X,Y}\left[1_{Y \neq f(X)}\right] &= \mathbb{E}_X\left[\mathbb{E}_{Y|X}\left[1_{Y\neq X}|X\right]\right] && (18)\\
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&\geq \mathbb{E}_X\left[\min_{y\in\mathcal{Y}} \Pr(Y \neq y|X)\right] && (20)\\
&= \mathbb{E}_X\left[\Pr(Y \neq f^\star(X)|X)\right] = \mathbb{E}_{X,Y}\left[1_{Y\neq f^\star(X)}\right] = L_{\mathcal{D}}(f^\star) && (21)
\end{aligned}
$$

Claim 2: $f^\star(\mathbf{x}) \in \arg\min_{y\in\mathcal{Y}} \Pr(Y \neq y|X = \mathbf{x})$

$$
f^\star(\mathbf{x}) \in \arg\max_{y\in\mathcal{Y}} \Pr(Y = y|X = \mathbf{x}) = \arg\min_{y\in\mathcal{Y}} \Pr(Y \neq y|X = \mathbf{x}) \qquad (22)
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  $\Rightarrow$ Follow nearest neighbors' decisions (KNN).

- **Parametric:** approximate true distribution $\mathcal{D}$ via training data
  $\Rightarrow$ Minimize the empirical risk on training data (ERM)

Recap

- Classification:
  - Mapping inputs to discrete outputs (categorical)
  - Not a special form of regression!
- Ways to perform classification:
  - **Non-parametric**: K-Nearest-Neighbors
  - **Parametric**: learning X-to-Y mapping via ERM
  - More complex decision boundaries? Non-linear classifiers

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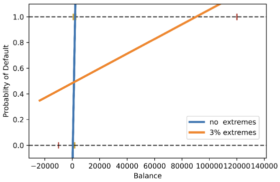

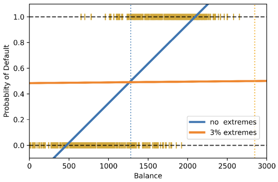

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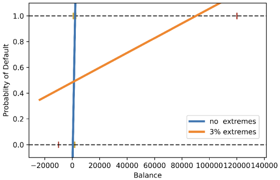
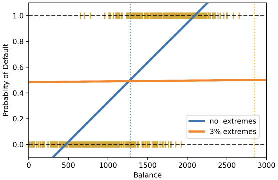
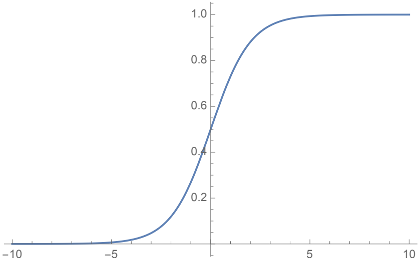




Solution: Transforming the predictions that take values in $(-\infty, \infty)$ into $[0, 1]$.

The logistic function

Consider first of all the case of two classes.



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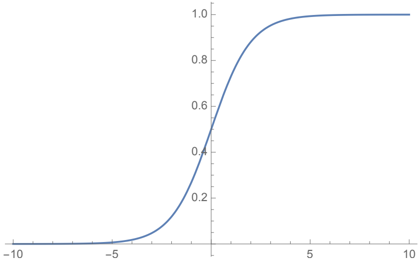

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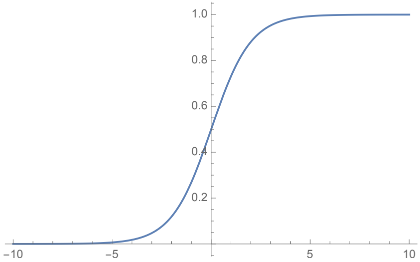

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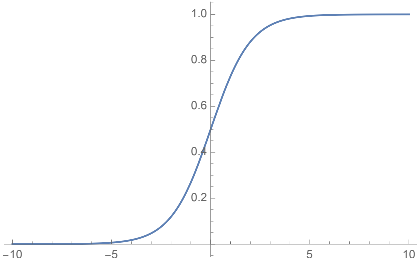

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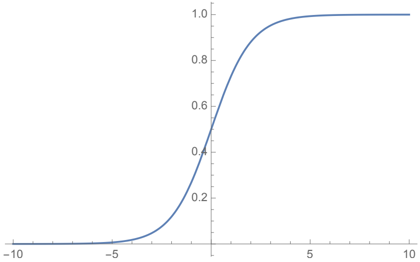

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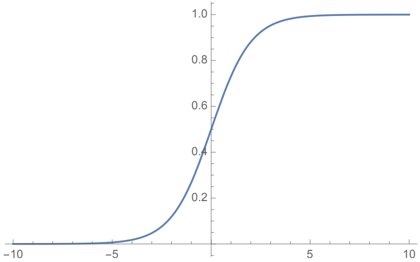

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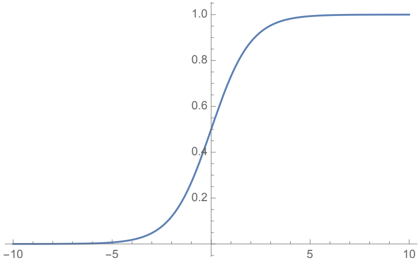

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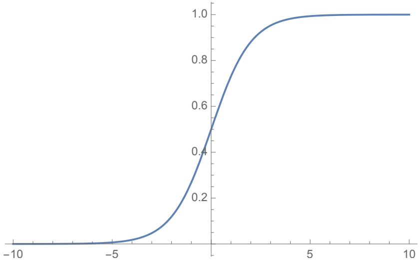

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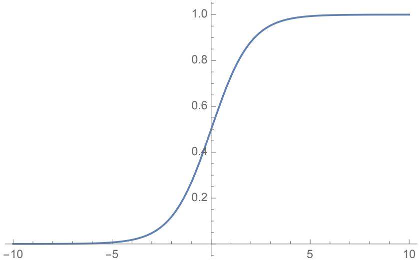

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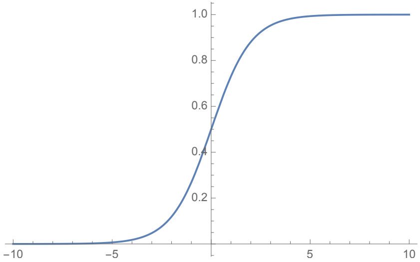

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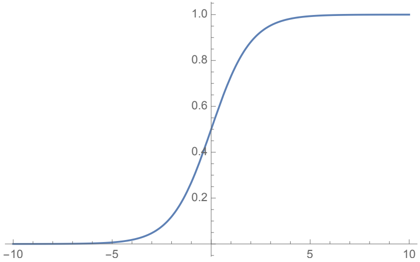

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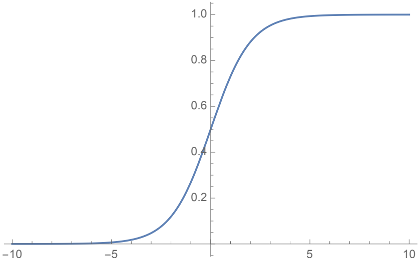

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Given a "new" feature vector $\mathbf{x}$, we predict the (posterior) probability of the two class labels given $\mathbf{x}$ by means of

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MLE for Logistic Regression

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As a result,

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Gradient of the negative log likelihood

Recall that

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$\Rightarrow$ Good news: the cost function L is convex.

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Second proof: Hessian of $\mathcal{L}$ is psd

The Hessian $\nabla^2\mathcal{L}$ is the **matrix** whose entries are the **second derivatives** $\frac{\partial^2}{\partial w_i \partial w_j}\mathcal{L}(\mathbf{w})$.

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$\Longrightarrow \mathcal{L}$ is convex since $\nabla^2\mathcal{L}(\mathbf{w}) \succeq 0$.