Classification with Linear Models

Losses for linear classification, logistic regression, multiclass classification

Machine Learning and Data Mining, 2024

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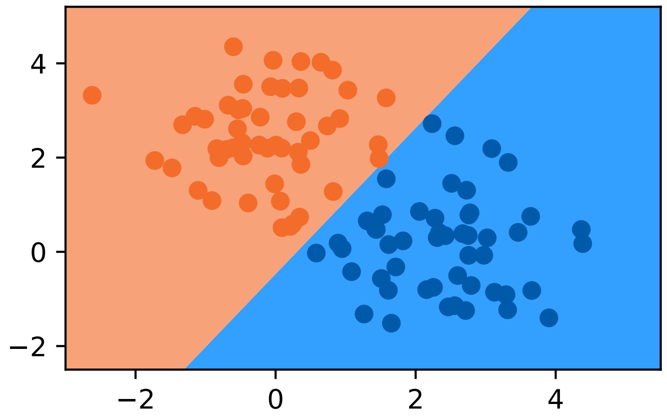
Can’t we just use linear regression for classification?

Classification with linear regression

Classification:

$$\hat{f}(x) = \mathrm{sign}[\theta^{\mathrm{T}} x]$$



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- $y = +1$ for **positive** class
- $y = -1$ for **negative** class

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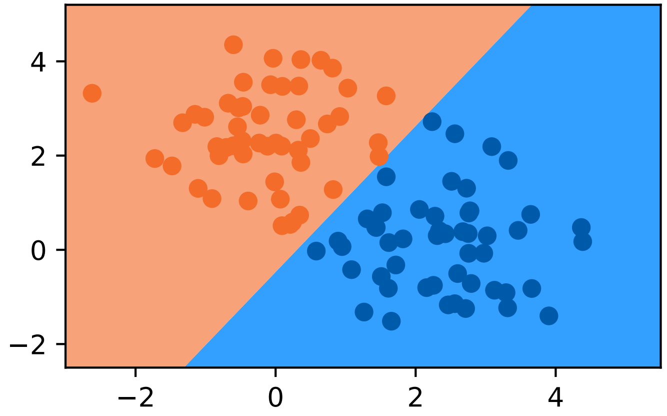

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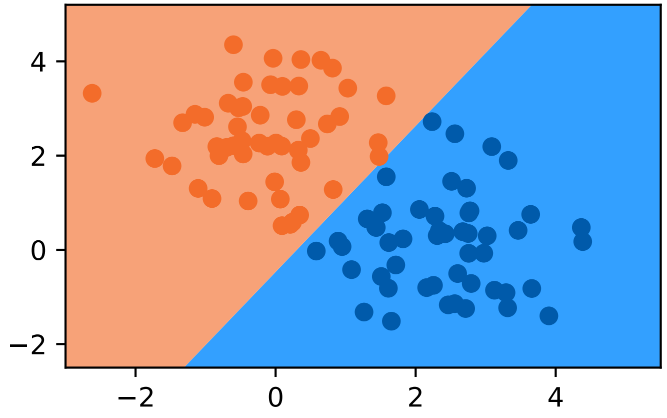

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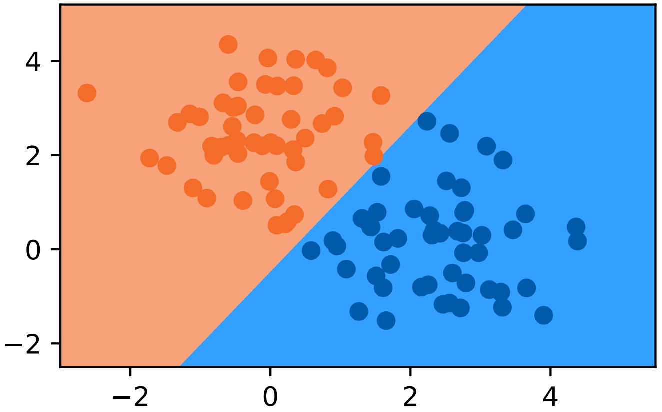

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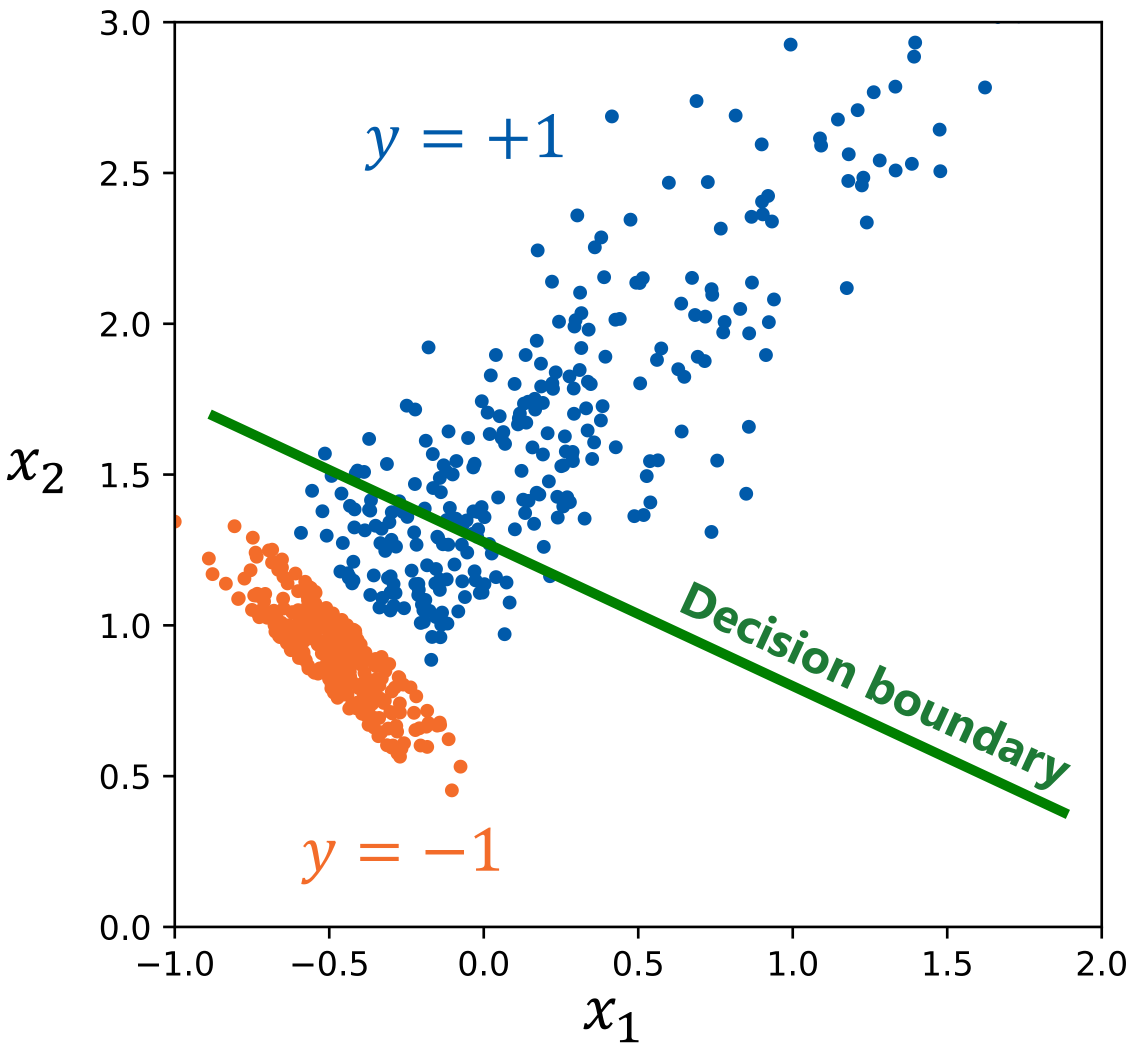
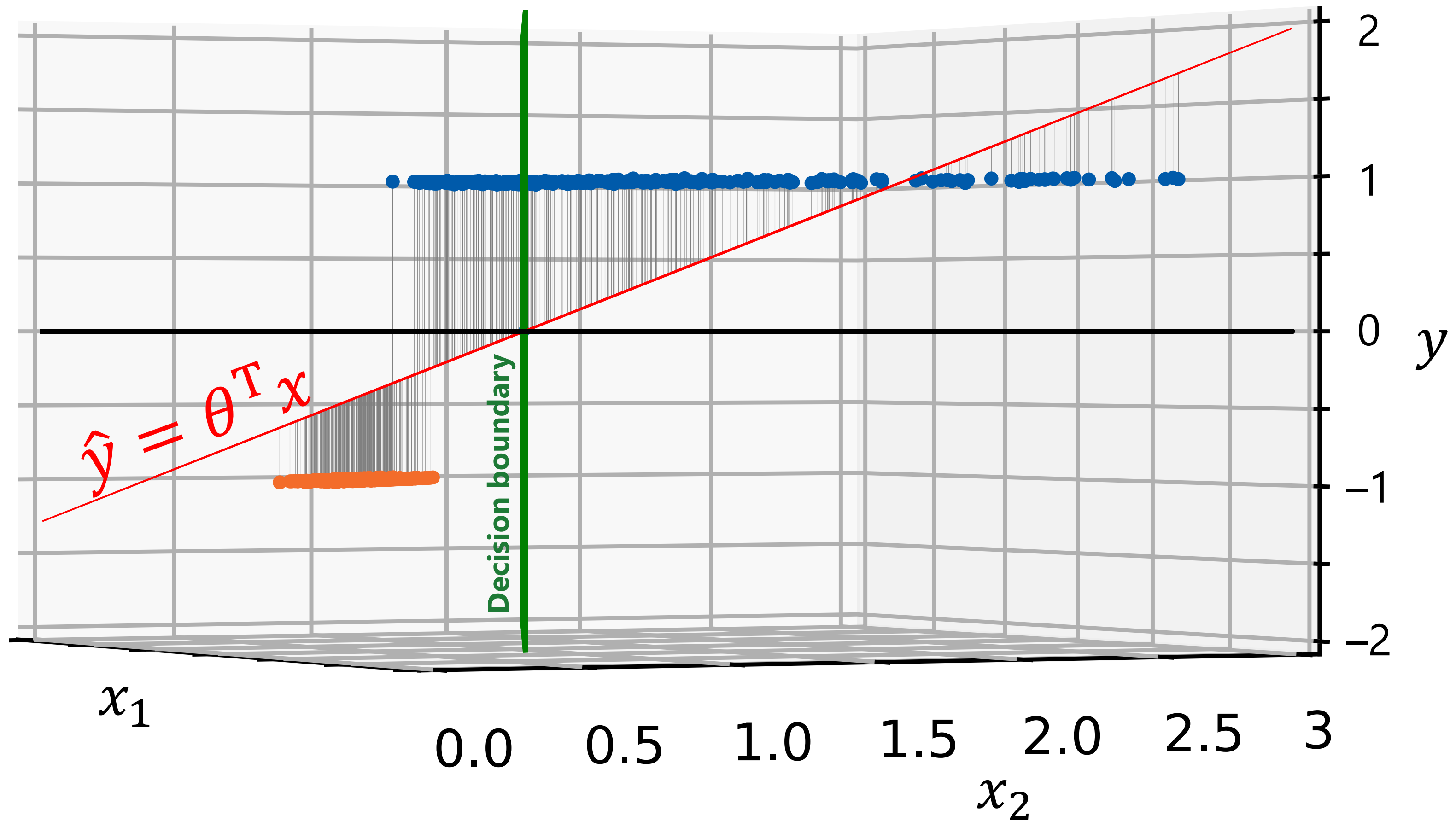
Any problems with this approach?

Classification with linear regression



May face problems when classes are unbalanced or have different spread

Classification with linear regression



MSE loss makes the model **avoid high residuals**

at a price of **pushing the decision boundary** towards the class with higher spread

Can we find a better loss function?

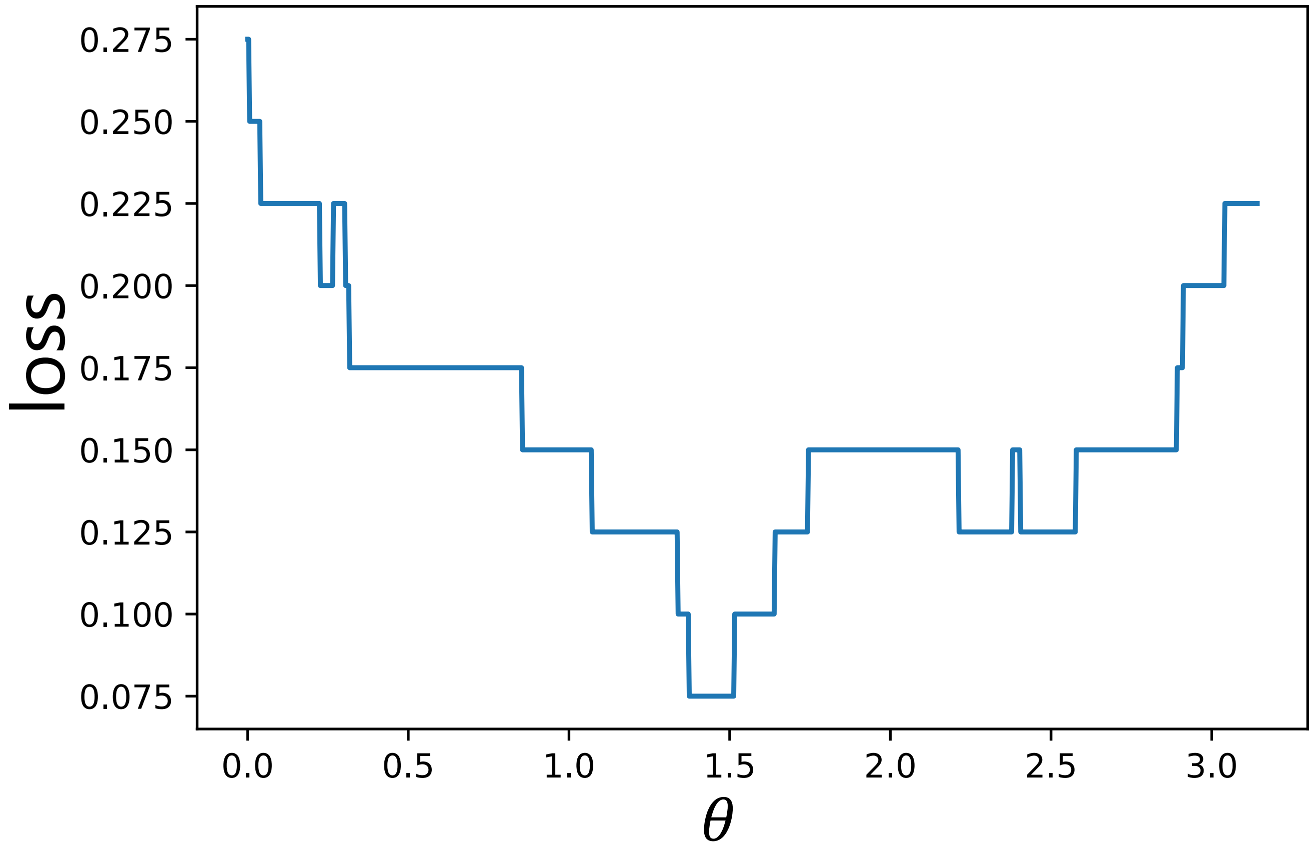
Classification loss functions

0-1 Loss

Probability of an error

$$\mathcal{L}_{0-1} = \frac{1}{N} \sum_{i=1...N} \mathbb{I}\left(\theta^{\mathrm{T}} x_i \cdot y_i < 0\right)$$

$$y_i \in \{-1, +1\}$$



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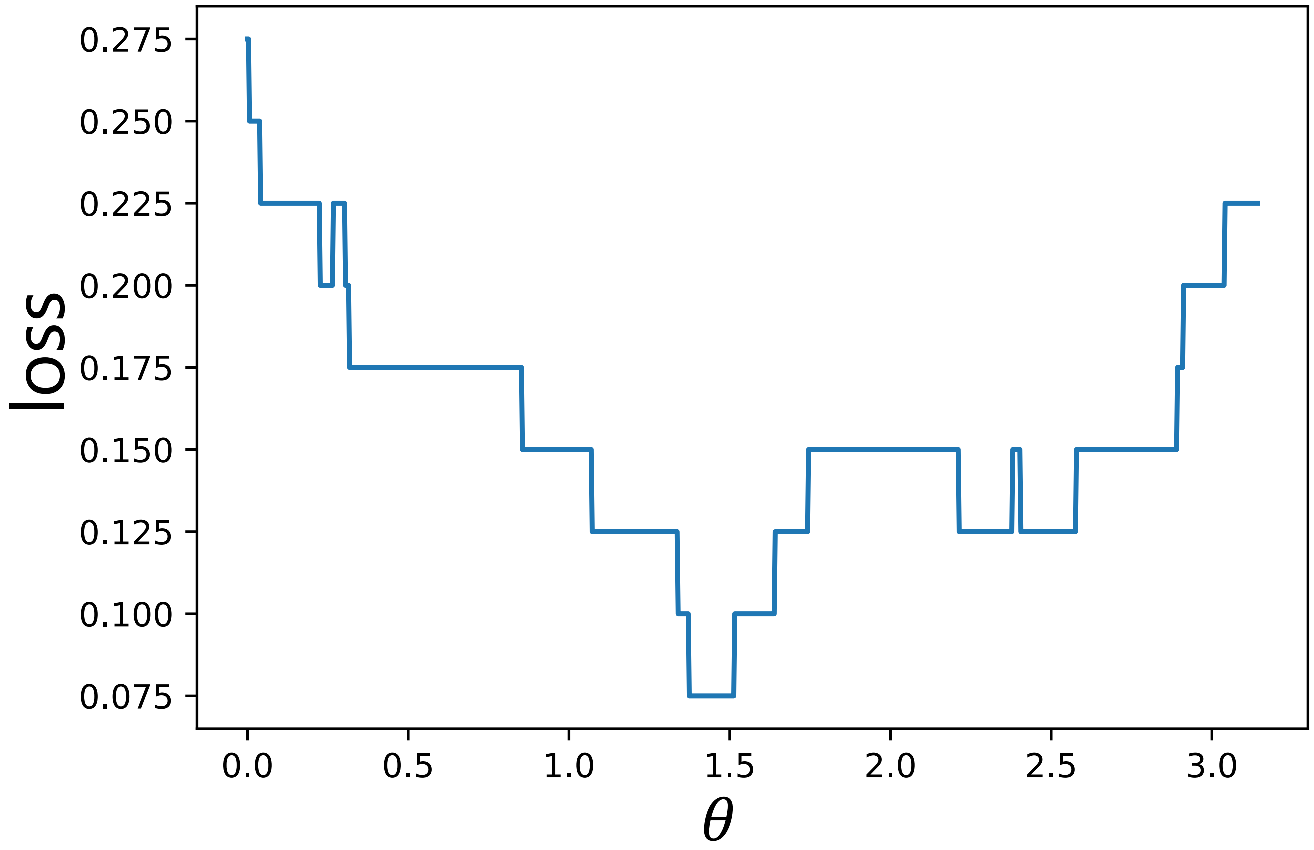


Can't optimize **piecewise constant** function with gradient-based methods*

*other techniques exist (still quite limited)

Margin

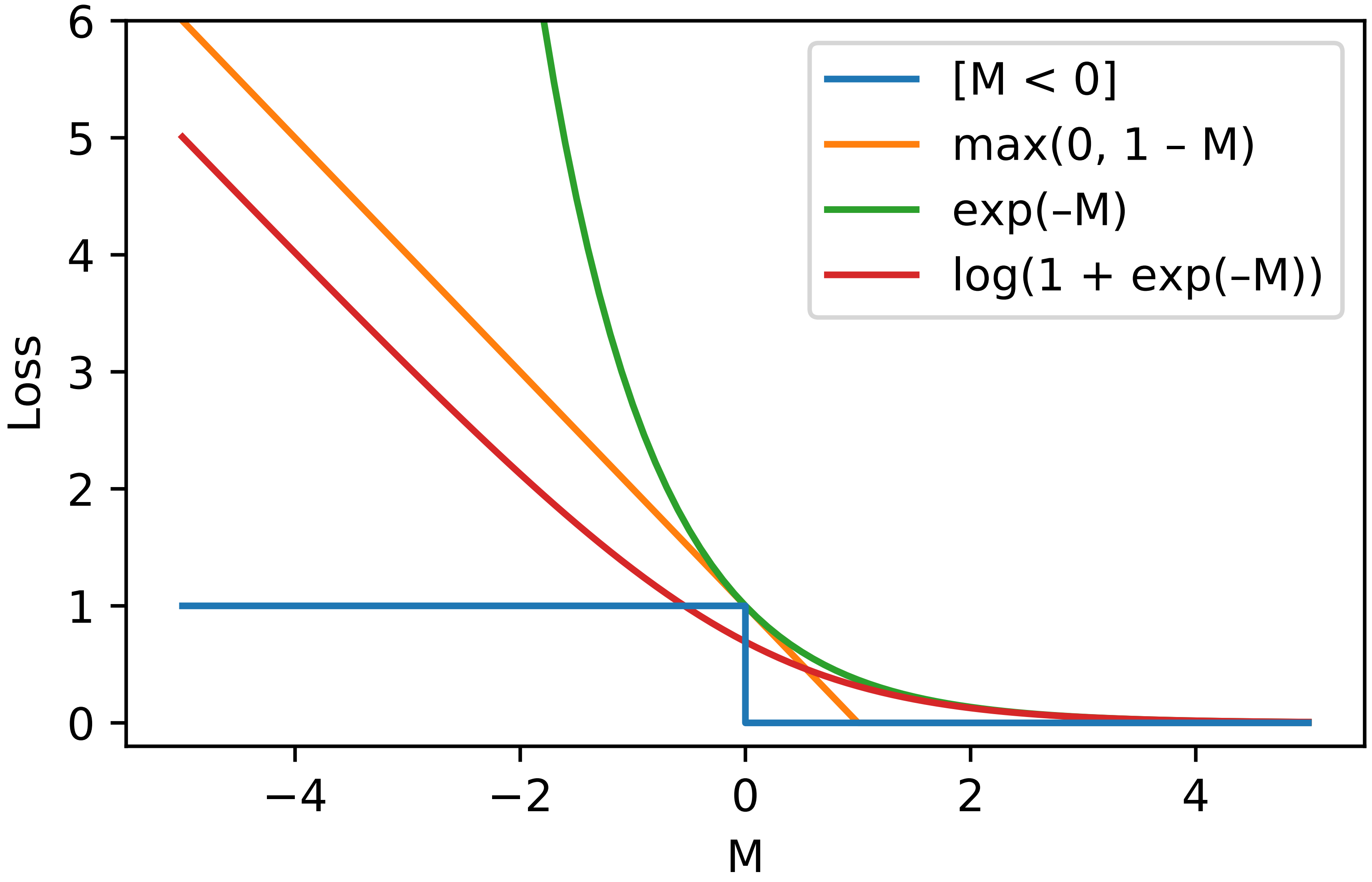
$$M = \theta^{\mathrm{T}} x \cdot y$$

$$\mathcal{L}_{0-1} = \frac{1}{N} \sum_{i=1 \dots N} \mathbb{I}\big(\underbrace{\theta^{\mathrm{T}} x_i \cdot y_i}_{\text{margin}} < 0\big)$$

$M > 0$ – correct classification

$M < 0$ – incorrect classification

Upper bounds on 0-1 loss



Instead of optimizing the 0-1 loss we can optimize a **differentiable upper bound**

Logistic Regression

Idea

Let's model the **class probabilities**

$$P(y = +1|x) = \widehat{f_\theta}(x)$$
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$$\text{Likelihood} = \prod_{i=1\ldots N} P(y_i|x_i)$$
$$= \prod_{i=1\ldots N} \left[\mathbb{I}[y_i = +1] \cdot \widehat{f_\theta}(x_i) + \mathbb{I}[y_i = -1] \cdot \left(1 - \widehat{f_\theta}(x_i)\right)\right]$$

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$$\theta = \underset{\theta}{\operatorname{argmax}} \sum_{i=1\ldots N} \left[\mathbb{I}[y_i = +1] \cdot \log \hat{f}_\theta(x_i) + \mathbb{I}[y_i = -1] \cdot \log\left(1 - \hat{f}_\theta(x_i)\right)\right]$$

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Predict the class with **highest probability***

*more generally: find a probability threshold suitable for your problem

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Common choice – **sigmoid function**:

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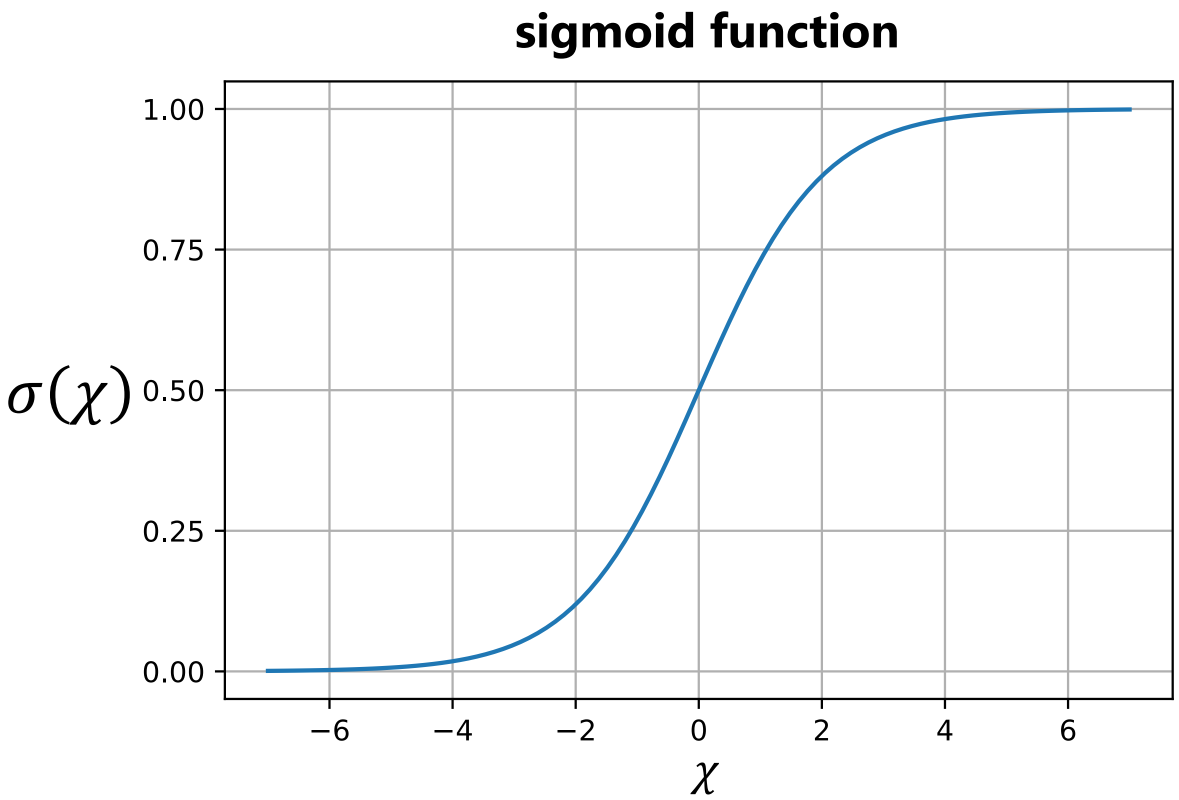

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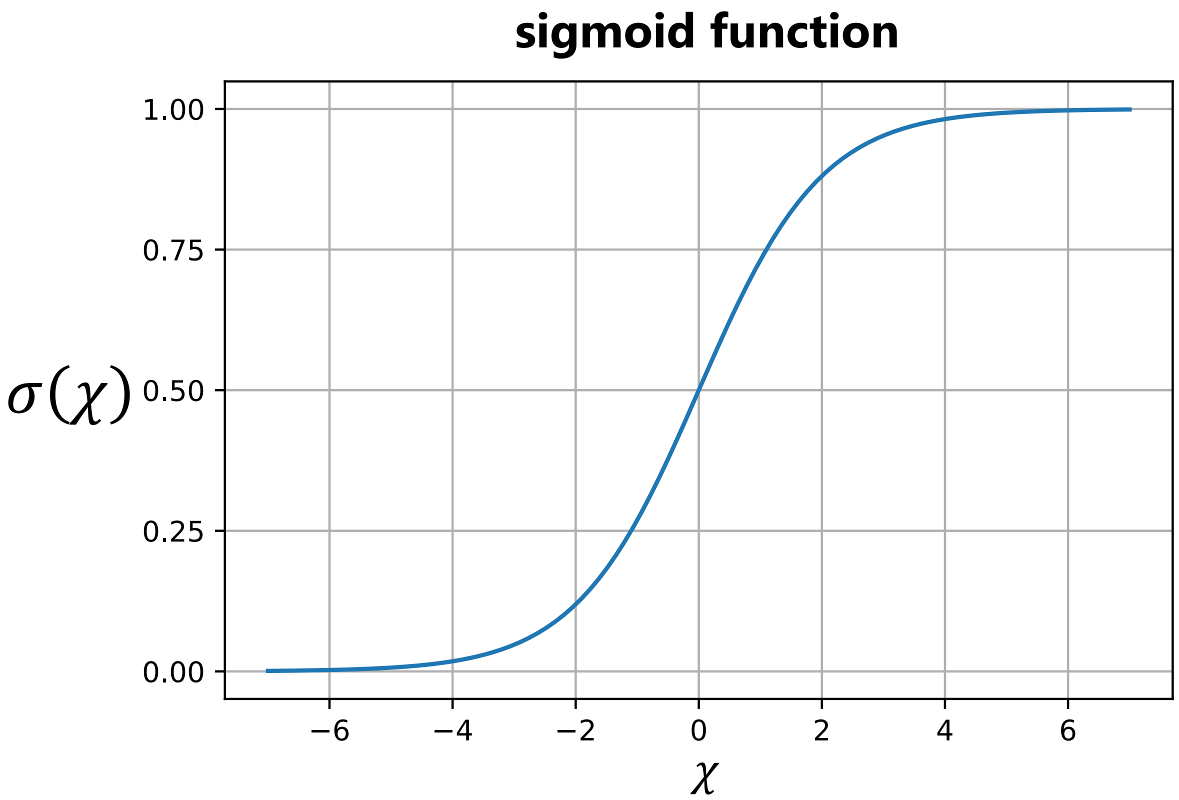

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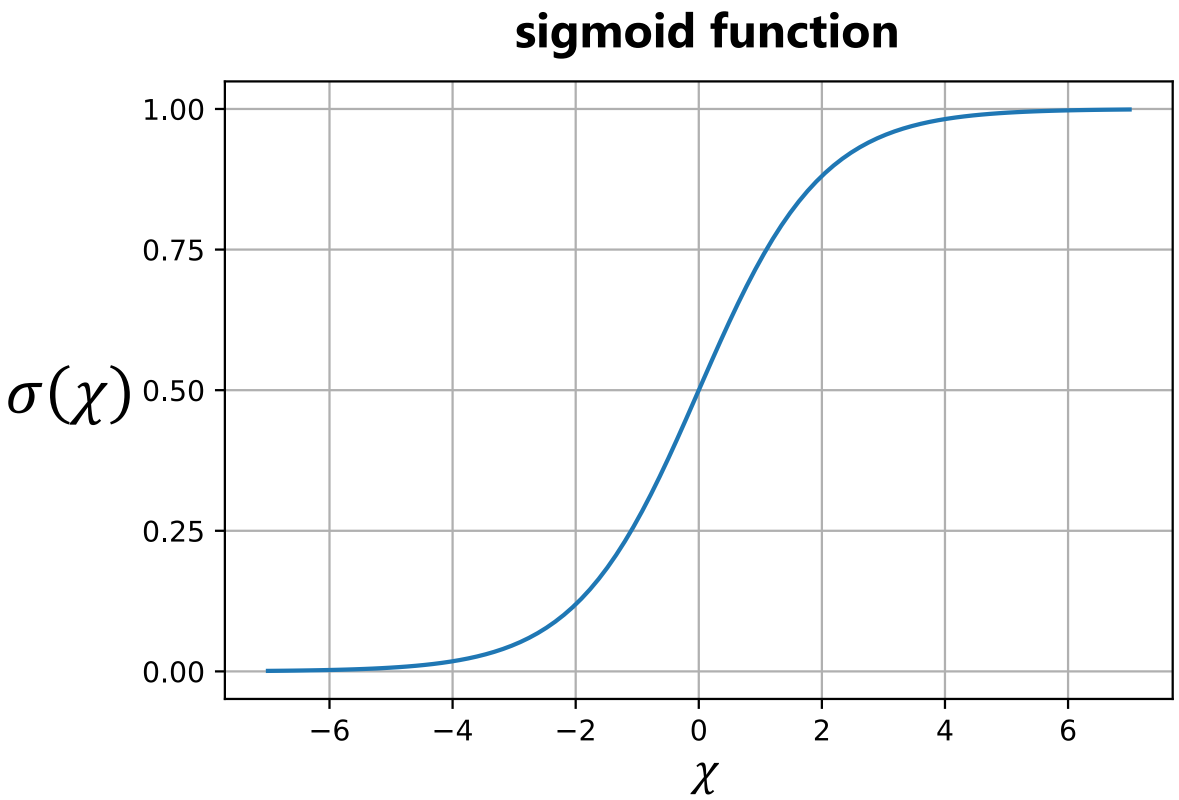
Then, $\theta^{\mathrm{T}} x$ has the meaning of **log odds ratio** between the two classes:



$$\log \frac{P(y = +1|x)}{P(y = -1|x)} = \log\left(\frac{1}{1 + e^{-\theta^{\mathrm{T}} x}} \cdot \frac{1 + e^{-\theta^{\mathrm{T}} x}}{e^{-\theta^{\mathrm{T}} x}}\right) = \theta^{\mathrm{T}} x$$

Bringing it all together

Use negative log likelihood as our loss function:

$$\mathcal{L} = -\sum_{i=1\dots N} \left[\mathbb{I}[y_i = +1] \cdot \log \widehat{f_\theta}(x_i) + \mathbb{I}[y_i = -1] \cdot \log\left(1 - \widehat{f_\theta}(x_i)\right) \right]$$

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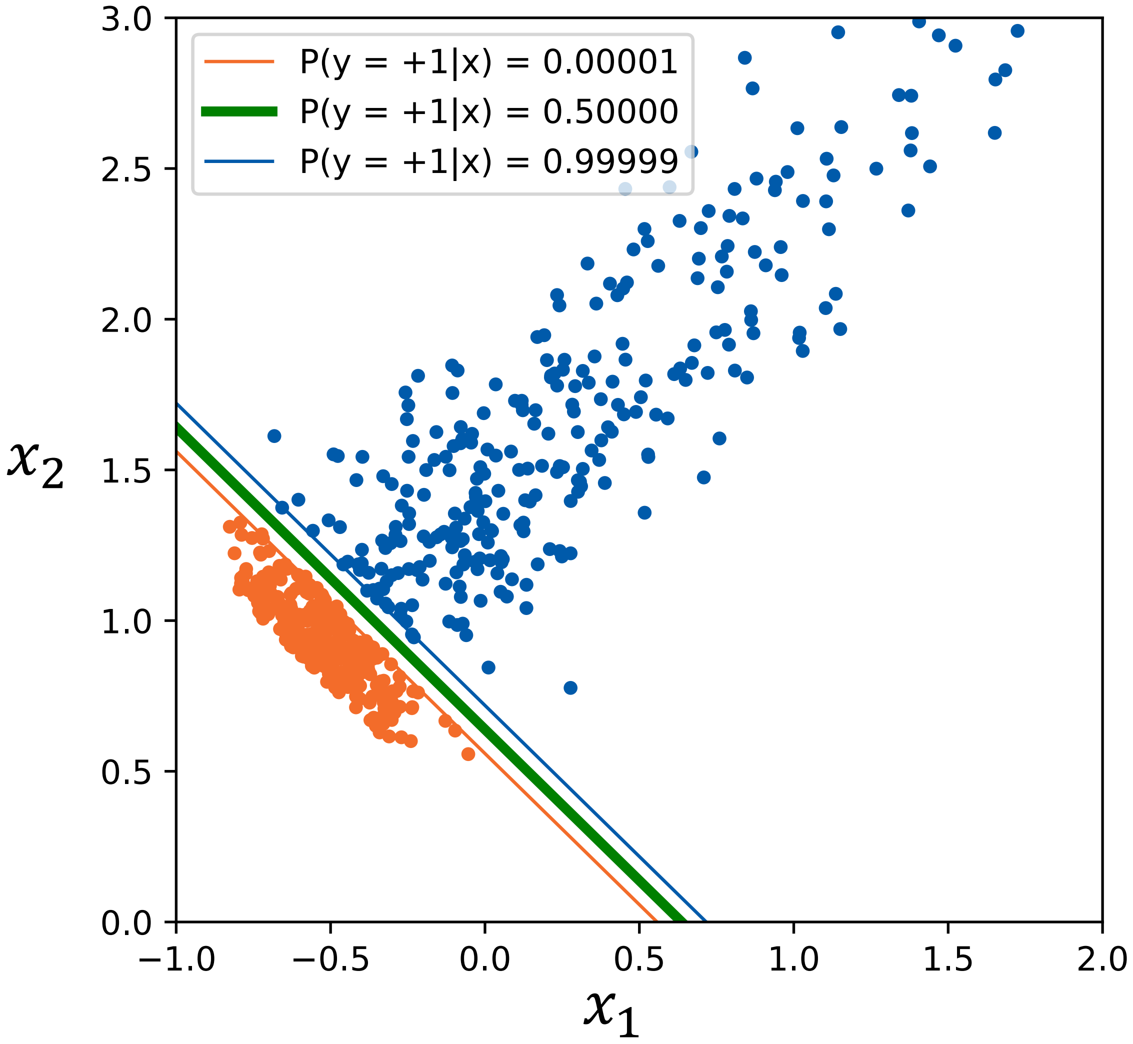
This can be optimized **numerically**

Example



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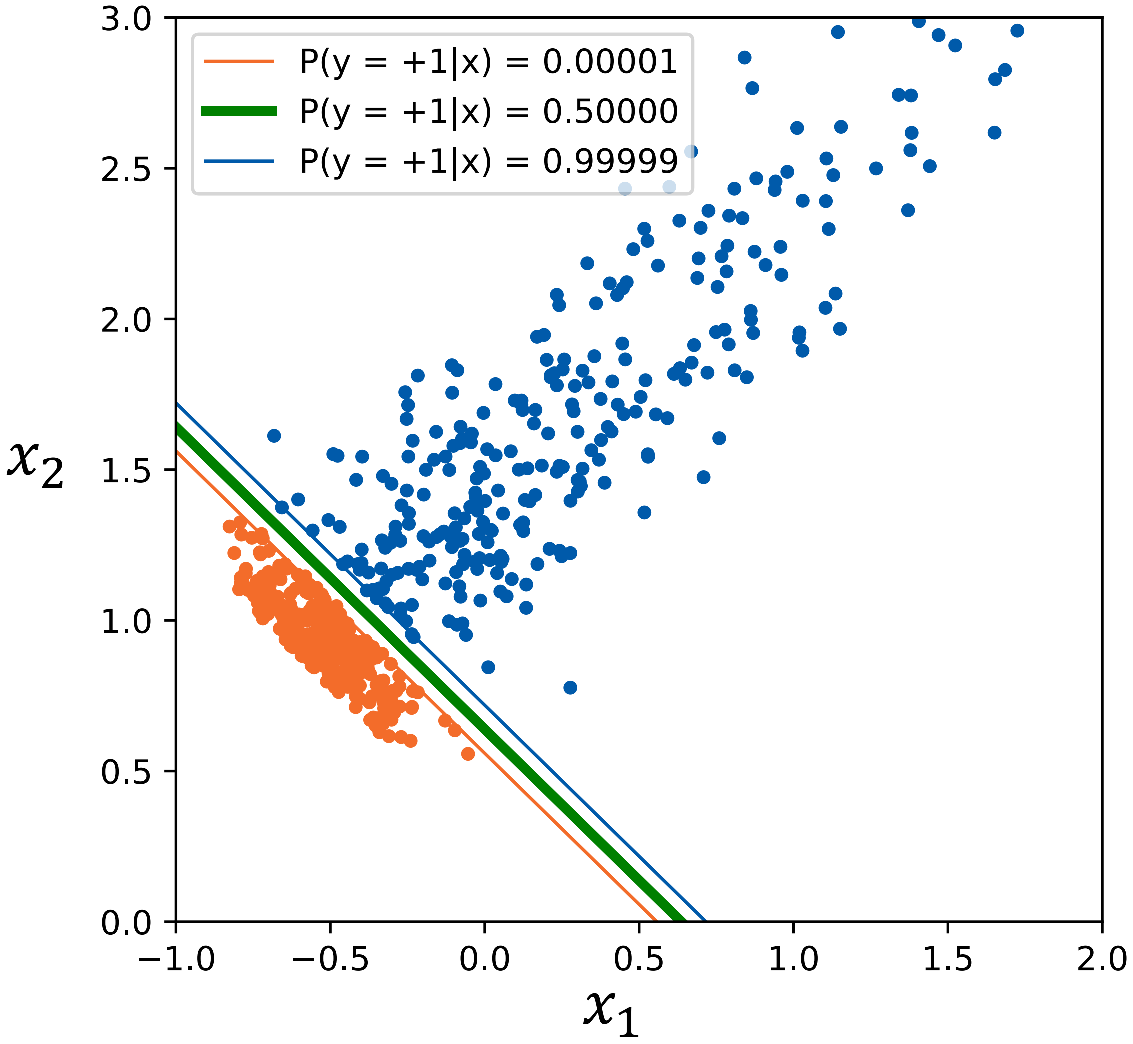

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$$\theta \longrightarrow C \cdot \theta, \text{ for some } C > 1 \in \mathbb{R}$$

keeps the boundary at the same place, yet improves the loss

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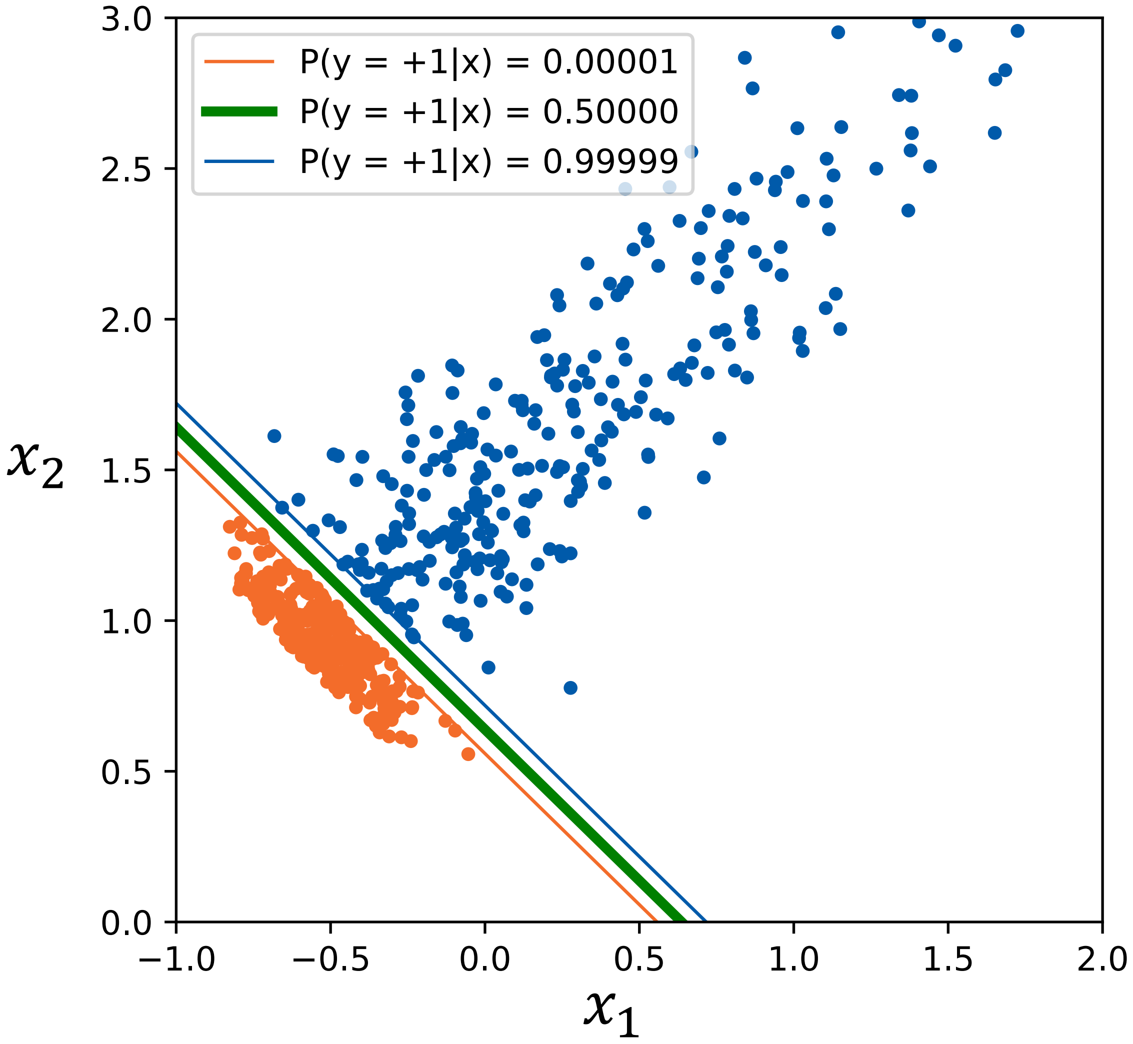

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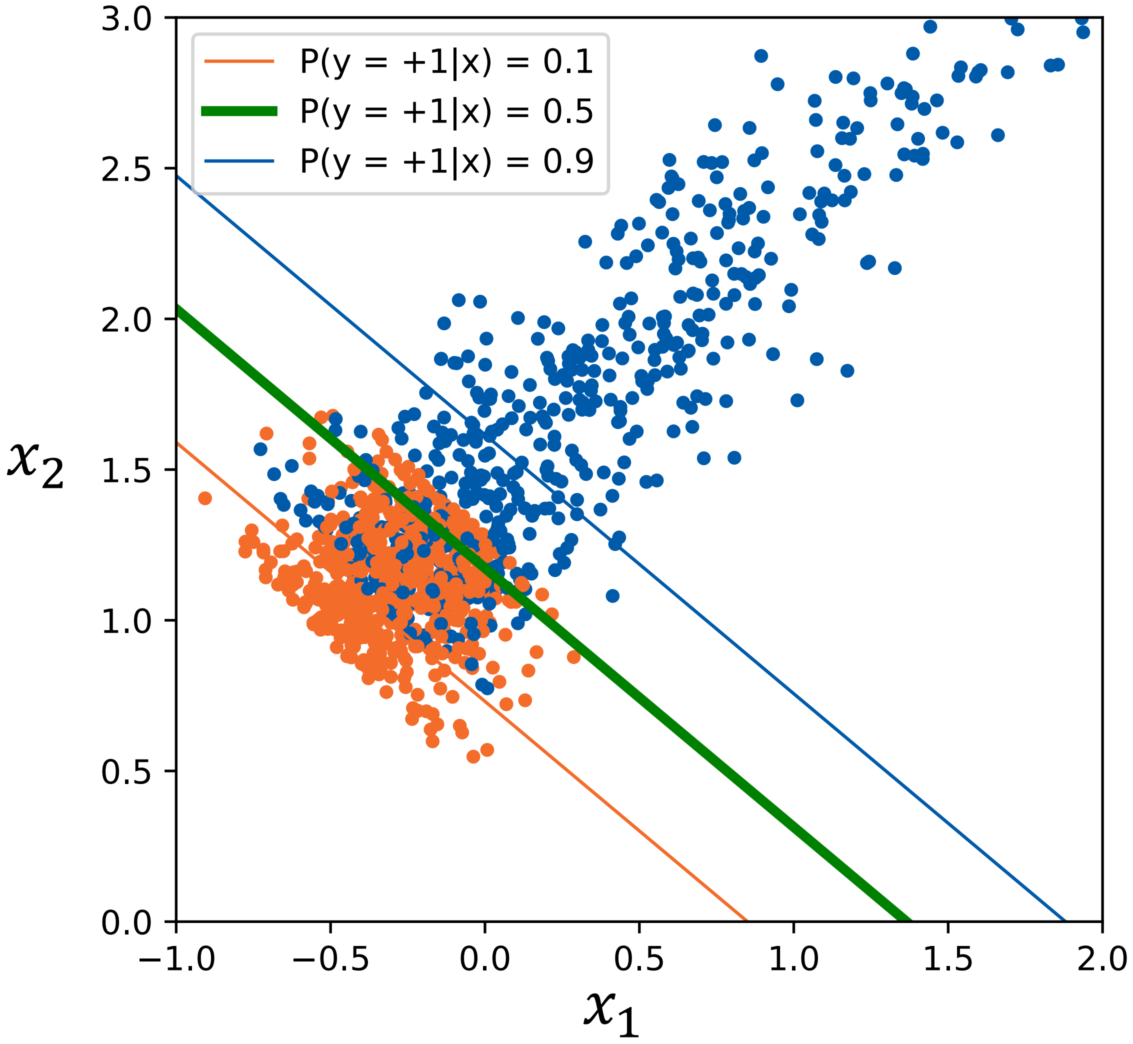
ideal fit when sigmoid turns into a step function (at infinitely large θ)

Example



When classes overlap the loss has a finite minimum

Predicted class probability changes smoothly

Multiclass Logistic Regression

Multinomial Logistic Regression

Similarly to the binary case, we'll model the class probabilities

Let's model **unnormalized** class probabilities like this:

$$\tilde{P}(y = k|x) = \exp \theta_k^{\mathrm{T}} x$$

Note: now we have K parameter vectors

Multinomial Logistic Regression

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Then, the **normalized** probabilities are:

$$P(y = k|x) = \frac{\tilde{P}(y = k|x)}{\sum_{k'=1\ldots K} \tilde{P}(y = k'|x)} = \frac{\exp \theta_k^{\mathrm{T}} x}{\sum_{k'=1\ldots K} \exp \theta_{k'}^{\mathrm{T}} x}$$

- This function is called **softmax** and is commonly used in neural networks

Multinomial Logistic Regression

Note that transforming all $\theta_k \longrightarrow \theta_k + v$ by some constant vector v does not affect the normalized probability

$$\tilde{P}(y = k|x) = e^{\theta_k^{\mathrm{T}} x} \longrightarrow e^{v^{\mathrm{T}} x} \cdot e^{\theta_k^{\mathrm{T}} x} = e^{v^{\mathrm{T}} x} \cdot \tilde{P}(y = k|x)$$

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This means we can **set one of the vectors $\boldsymbol{\theta_k}$ to 0**, e.g. the last one:

$$\theta_K = 0$$

Multinomial Logistic Regression

We now have $K - 1$ parameter vectors

Individual linear outputs $\theta_k^{\mathrm{T}} x$ now have the meaning of **log odds ratio** between the classes k and K:

$$\log \frac{P(y = k|x)}{P(y = K|x)} = \log \frac{\tilde{P}(y = k|x)}{\tilde{P}(y = K|x)} = \log \frac{e^{\theta_k^{\mathrm{T}} x}}{e^0} = \theta_k^{\mathrm{T}} x$$

Multinomial Logistic Regression

Plugging everything into the negative log likelihood we get our loss function:

$$\mathcal{L} = -\sum_{i=1\ldots N} \log \frac{\exp \theta_{y_i}^{\mathrm{T}} x_i}{1 + \sum_{k'=1\ldots K-1} \exp \theta_{k'}^{\mathrm{T}} x_i}$$

$$(\theta_K = 0)$$

Again, this can be optimized **numerically**

Multiclass classification: general approach

General idea

For a problem with K classes introduce K predictors:

$$\widehat{f_k}(x)\colon \mathcal{X} \to \mathbb{R}, \text{ for } \mathrm{k} = 1, \dots, K$$

each of which outputs a corresponding **class score**.

Predict the class with the **highest score**:

$$\hat{y}_i = \operatorname*{argmax}_k \widehat{f_k}(x_i)$$

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For each class k train a binary model $\widehat{f_k}(x) = \theta_{(k)}^{\mathrm{T}} x$ separating the given class from all others, $\hat{y}_{(k)}^{\mathrm{1-vs-rest}} = \mathrm{sign}\left[\widehat{f_k}(x)\right]$

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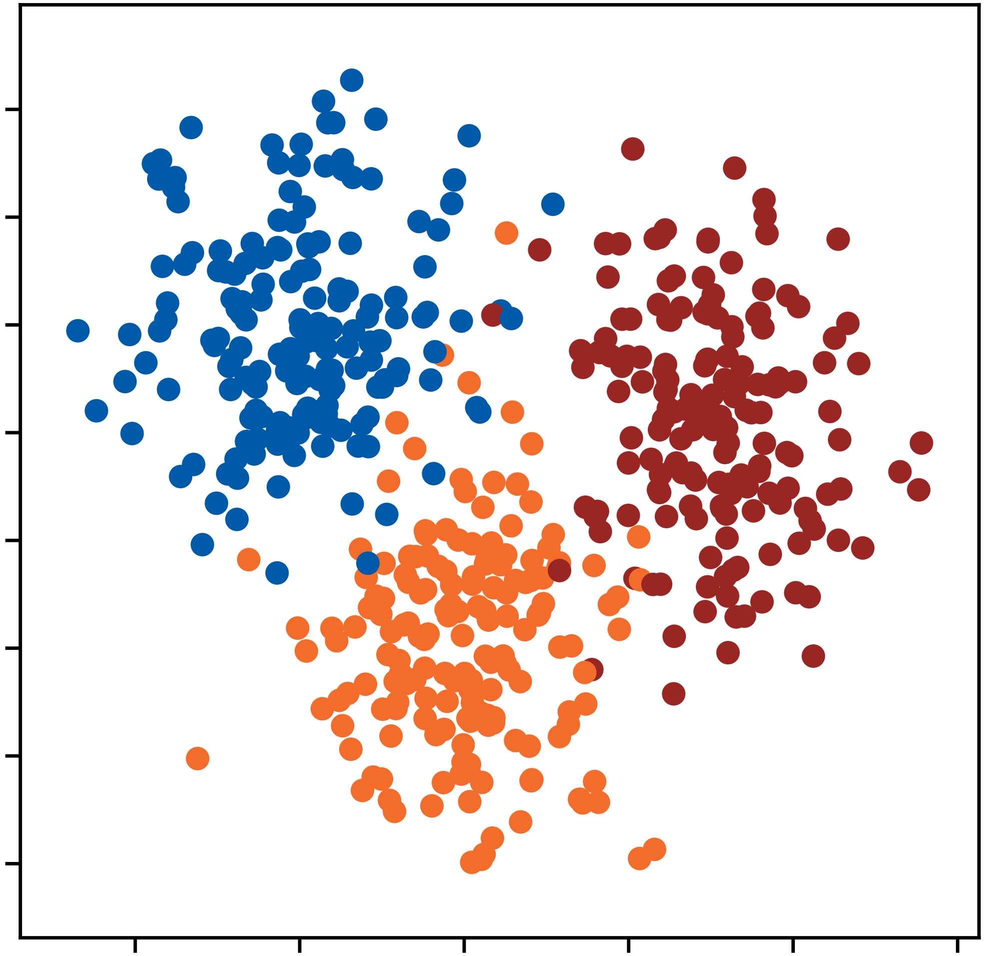
Use the outputs of $\widehat{f}_k$ as class scores for multiclass classification:

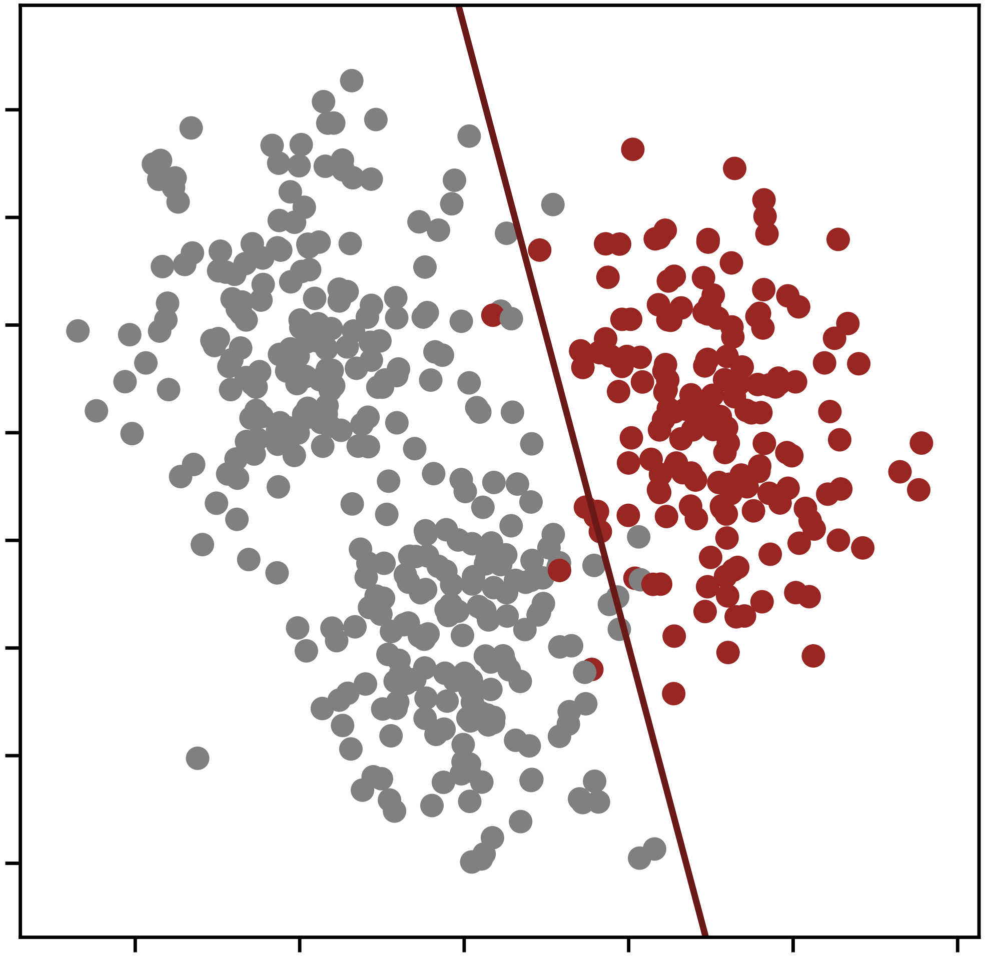
$$\hat{y}_i = \underset{k}{\mathrm{argmax}}\, \widehat{f}_k(x_i)$$

Example



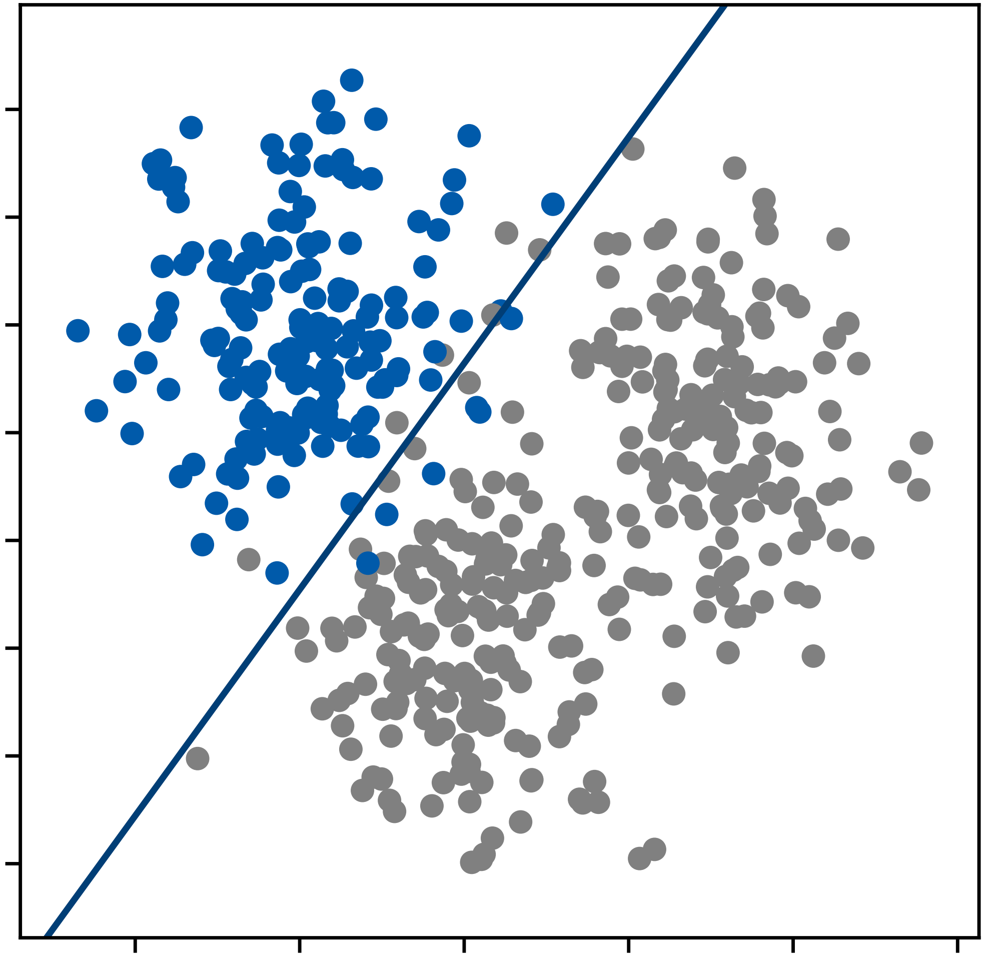
Consider the following 3 class problem

Example



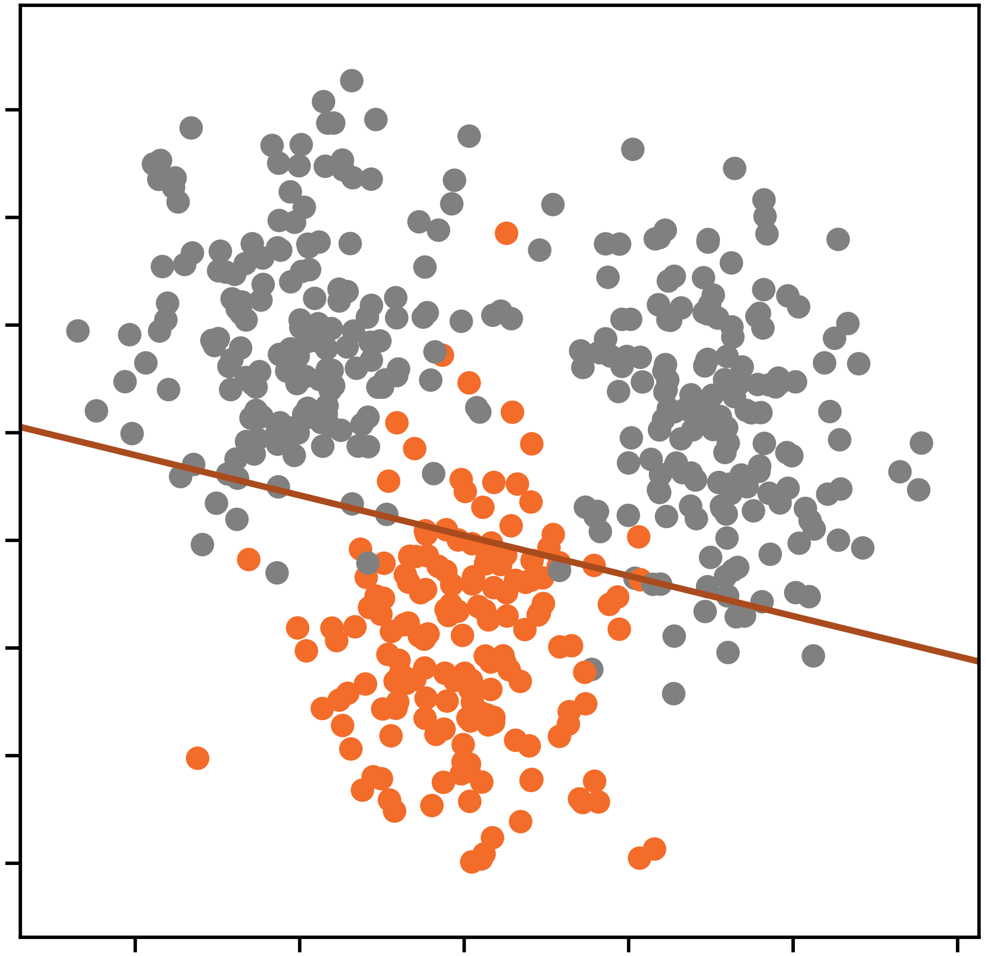
"Class-1 VS rest" binary classifier

Example



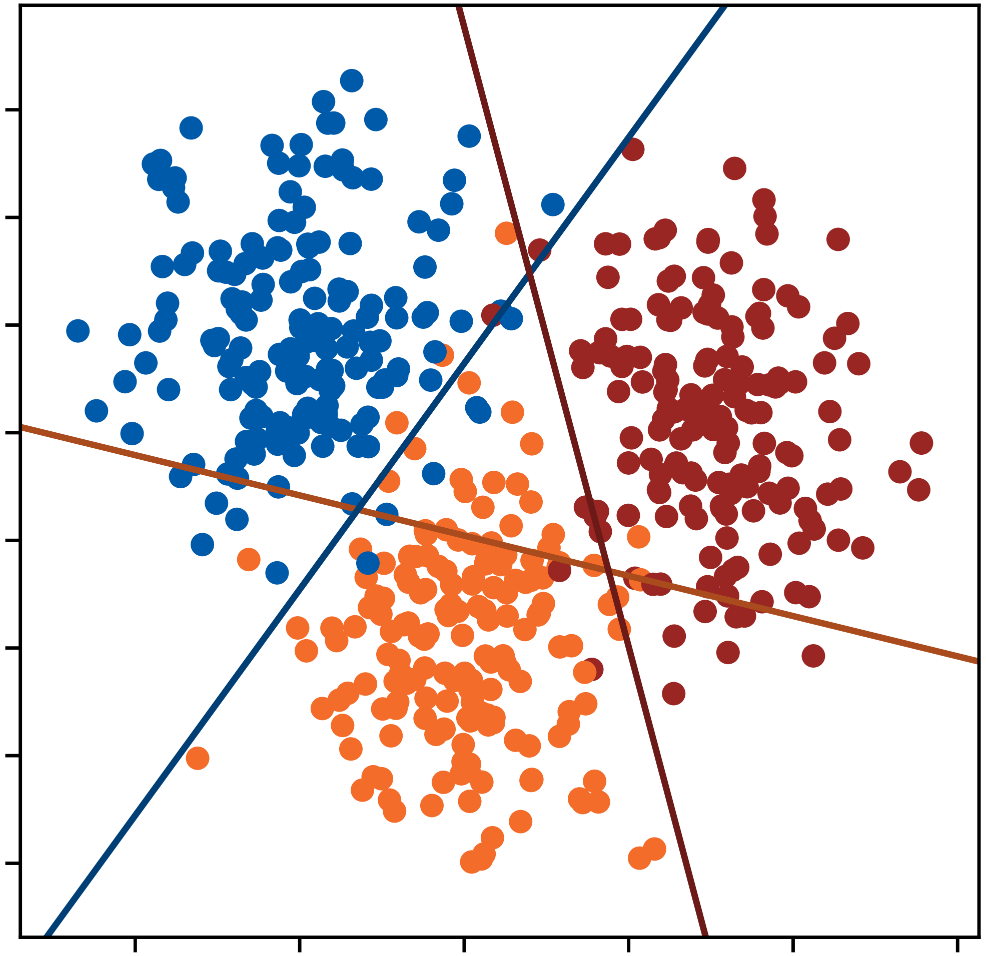
“Class-2 VS rest” binary classifier

Example



“Class-3 VS rest” binary classifier

Example



$\widehat{f}_k(x) = 0$ lines (binary decision boundaries)

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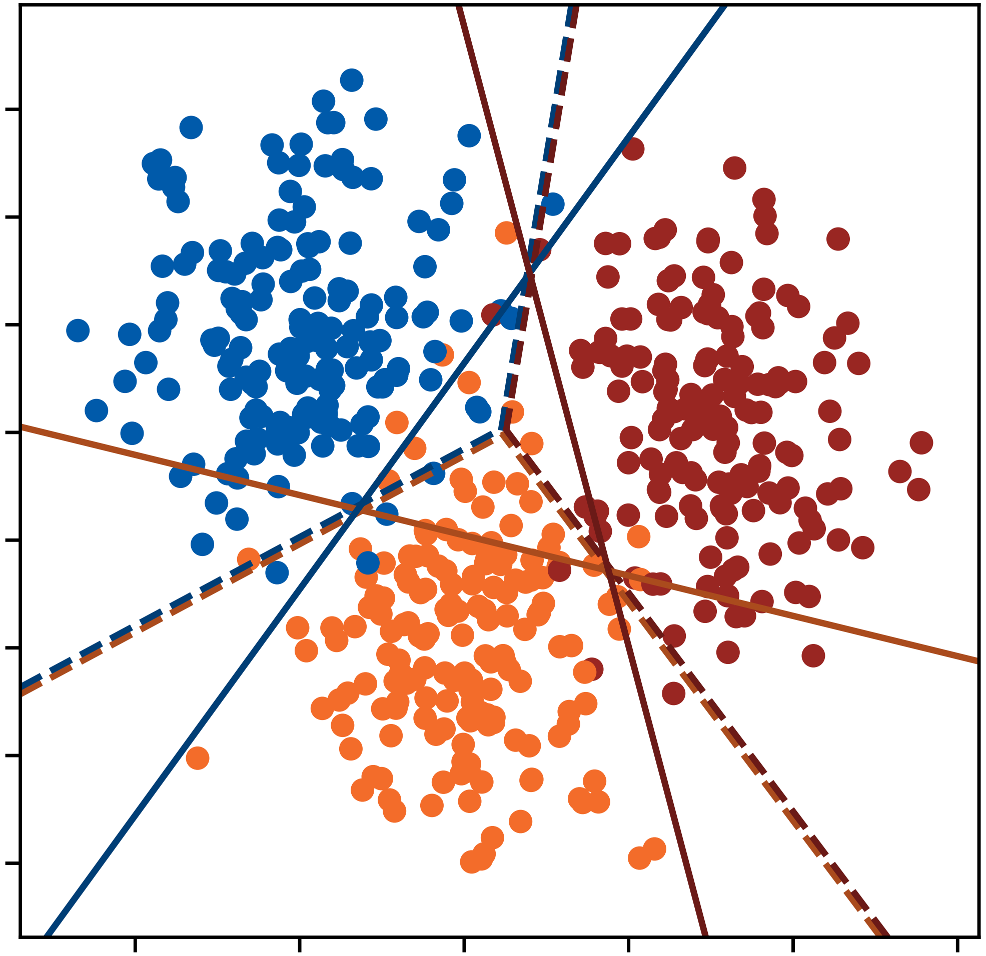

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Adding decision boundaries for

$\hat{y} = \underset{k}{\operatorname{argmax}} \widehat{f_k}(x)$

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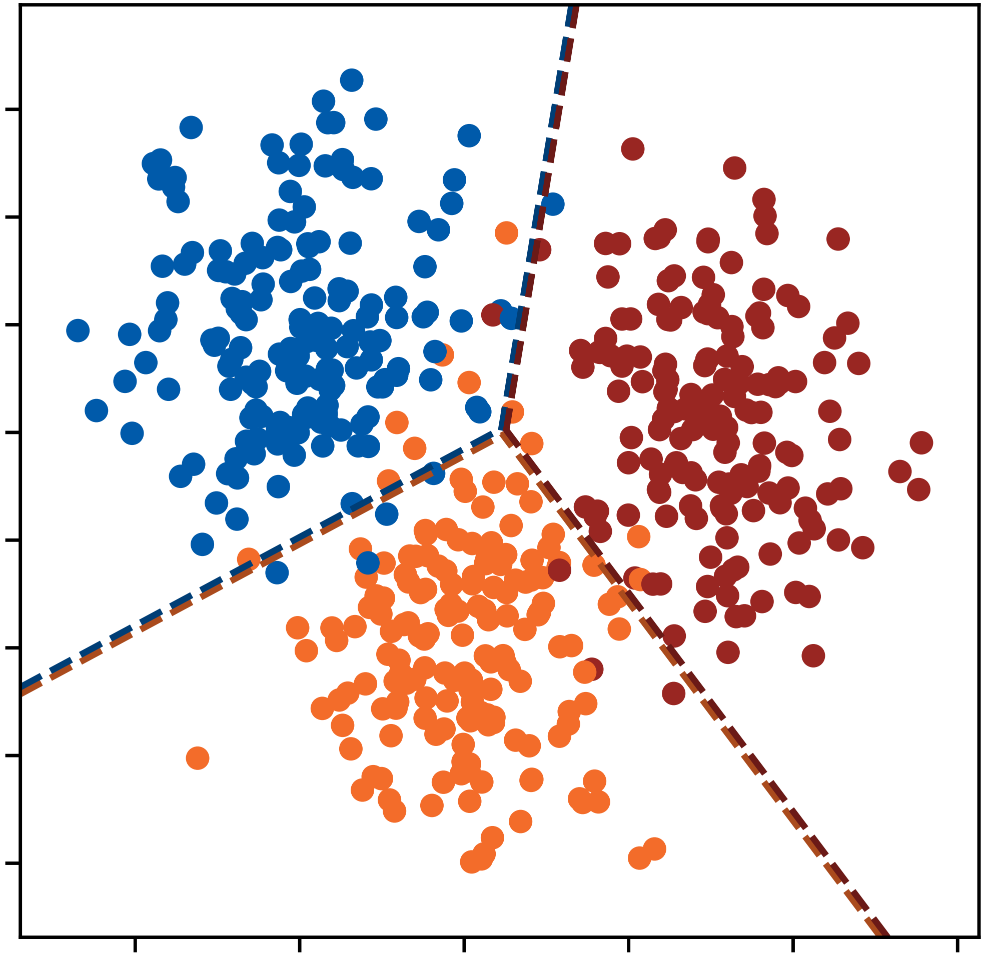

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Any binary linear classifier can be adapted to multiclass with the **one-vs-rest strategy**

Food for thought: how can you mitigate the biased probability problems when using one-vs-rest strategy (as discussed on the previous slide)?

Thank you!

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