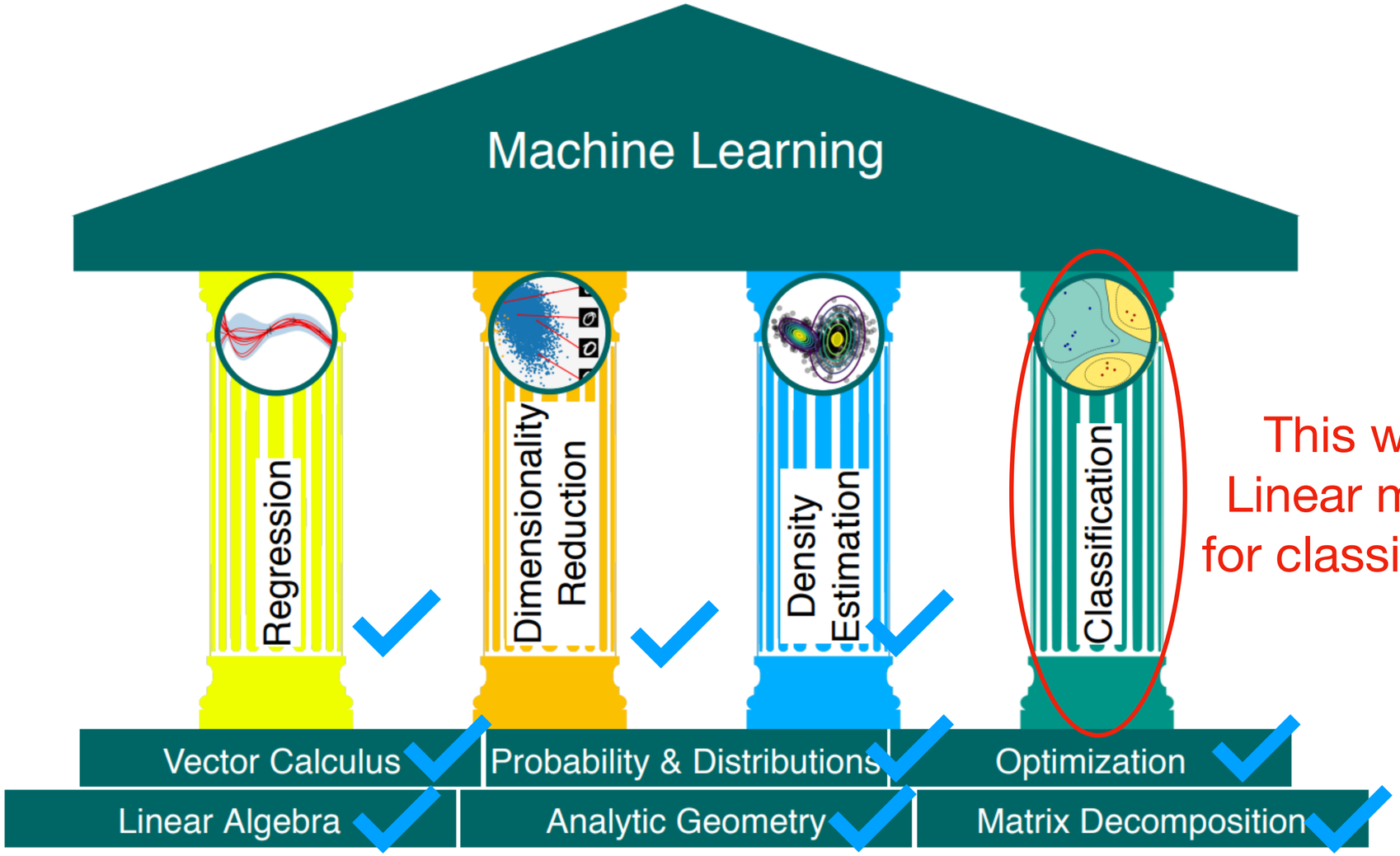
Classification

Week 11 - Introduction to ML / Thang Bui / ANU / 2023 S2

Housekeeping

- *Assignment 4* is now available on Wattle (due next week - W12 Monday)
- *No more* tutorials
- *Exam* timetable is available
  - Past exam papers released on Wattle
- Guest lecture: W12 Monday October 23
  - Dr Zheng Yuan, King's College London
  - *Examinable*!
  - Please do show up!

Foundations of ML



This week:
Linear models
for classification

Source: Maths for ML Textbook

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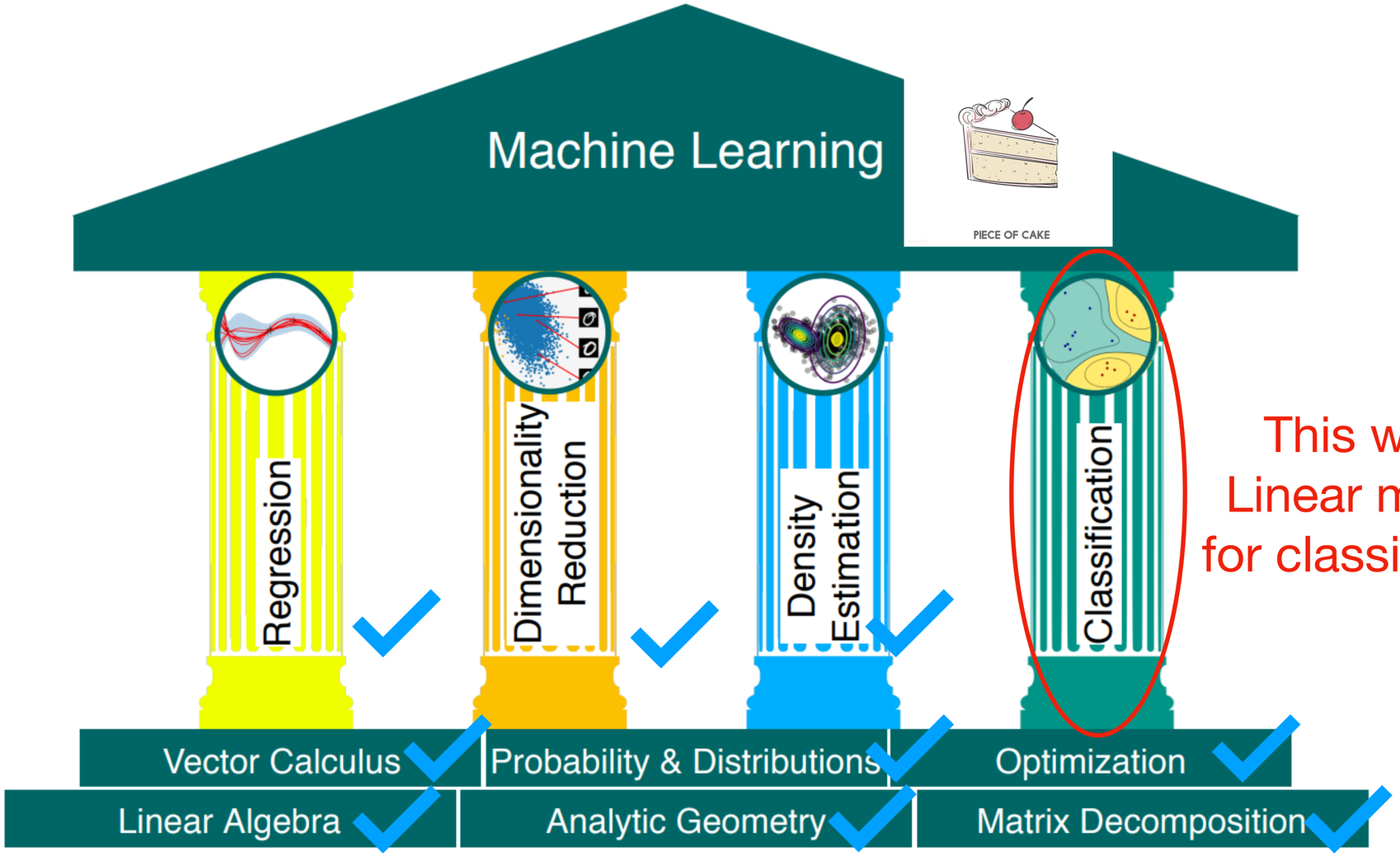

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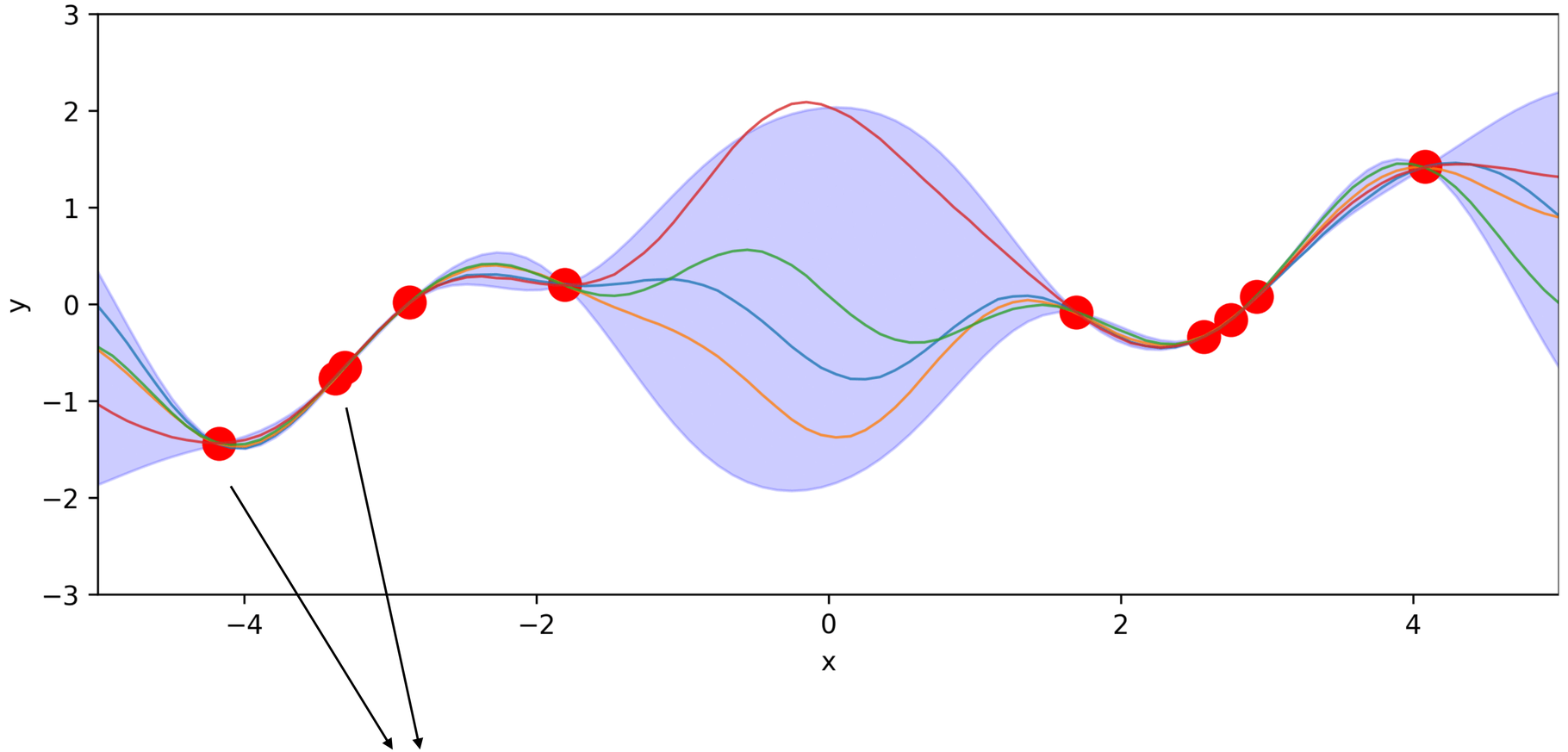
Overview

1. **Recap: Linear regression**
2. From least squares to binary logistic classification
3. From binary to multi-class classification
4. Evaluation
5. Linearly separable data - perceptron algorithm

Recap: regression and linear regression



Observed data

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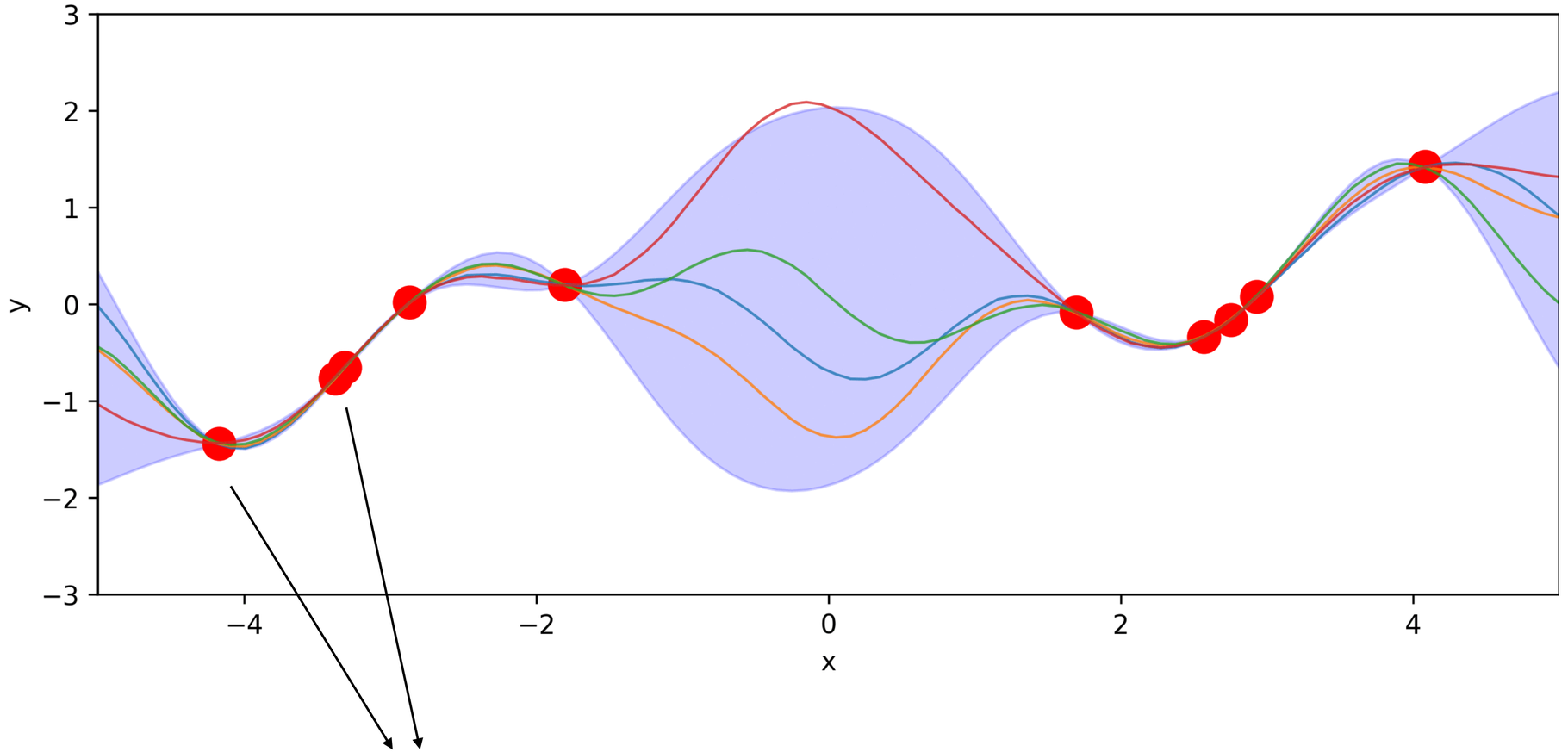

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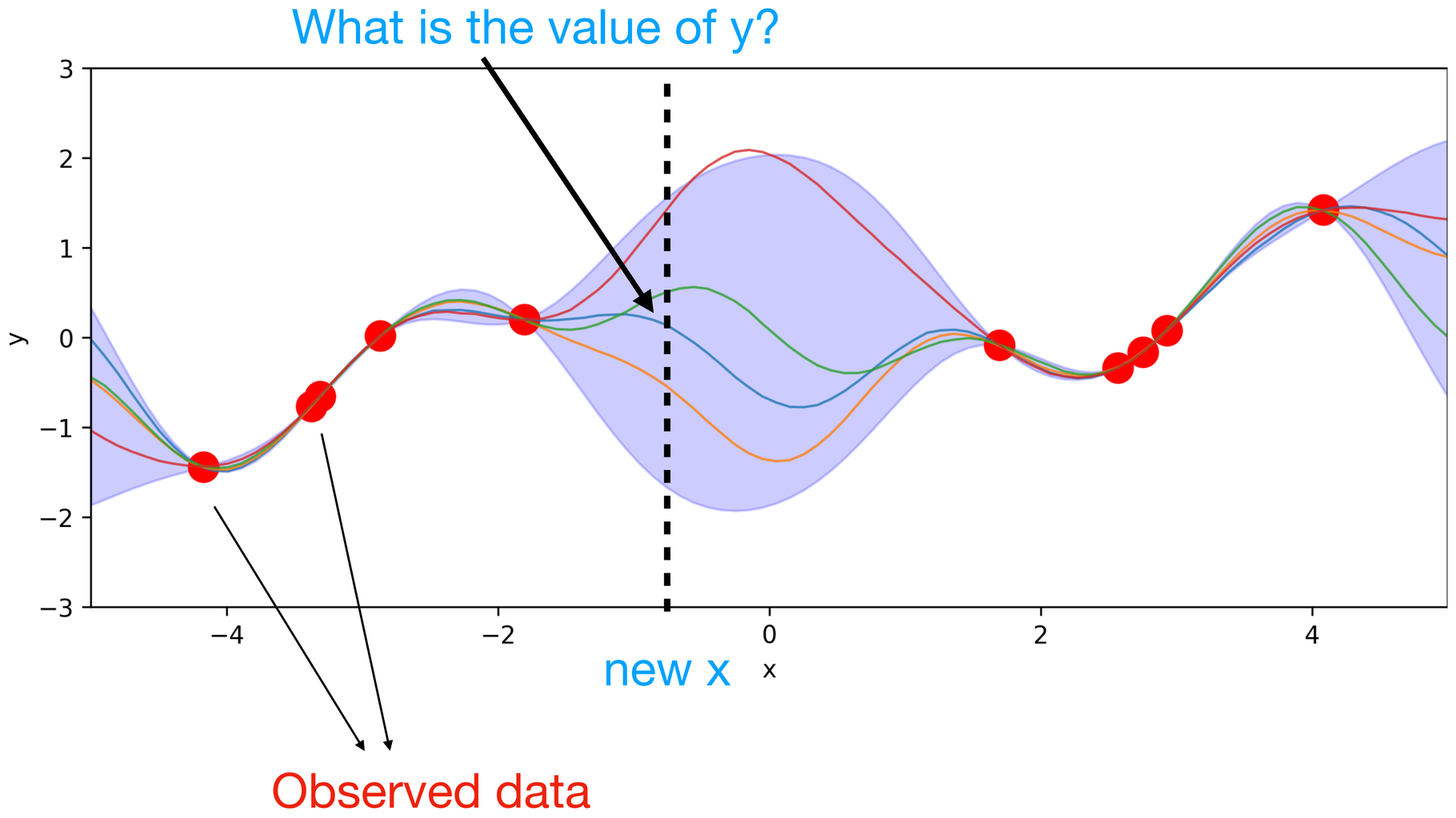

Data and linear assumption

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Training data N input, output pairs $\mathcal{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}, \mathbf{x}_n \in \mathbb{R}^D, y_n \in \mathbb{R}$

Each row is a data point

Each column is a feature dimension

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

One scalar per data point

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Test time: given a new input $\mathbf{x}^*$, prediction = $f(\mathbf{x}^*) = \theta^\intercal \mathbf{x}^*$

Objective function

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Loss function: $L(\theta) = \frac{1}{N} \sum_{n=1}^{N} (y_n - f_\theta(\mathbf{x}_n))^2 = \frac{1}{N} \|\mathbf{y} - X\theta\|_2^2 = \frac{1}{N} (\mathbf{y} - X\theta)^\intercal (\mathbf{y} - X\theta)$

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We want to find θ that minimises the loss function. Closed-form analytic solution!

$$\theta = (X^\intercal X)^{-1} X^\intercal \mathbf{y}$$

Regularised least squares

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Overfitting occurs because the model is too **complex** (θ has too many large entries), while there are too limited training sample.

We want to *penalise* the amplitude of parameters by **regularisation.**

Regularised least squares = least squares + regularisation

$$L_\lambda(\theta) = \frac{1}{N}\sum_{n=1}^{N}(y_n - f_\theta(\mathbf{x}_n))^2 + \lambda\|\theta\|_p^p$$

Data-fit
Lower = better fit

Regulariser
Lower = simpler model

Hyperparameter

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Loss function when p = 2: $L(\theta) = \frac{1}{N}\|\mathbf{y} - X\theta\|_2^2 + \lambda\|\theta\|_2^2 = \frac{1}{N}(\mathbf{y} - X\theta)^\intercal(\mathbf{y} - X\theta) + \lambda\|\theta\|_2^2$

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The probabilistic perspective

Week 6

Bayes' rule: $P(\theta \mid \mathscr{D}) = \frac{P(\theta, \mathscr{D})}{P(\mathscr{D})} = \frac{P(\theta)\, P(\mathscr{D} \mid \theta)}{P(\mathscr{D})}$

Posterior
belief about θ after knowing $\mathscr{D}$

$=$

$$\frac{\textbf{Prior}\ \text{prior belief about } \theta \quad \times \quad \textbf{Likelihood}\ \text{likelihood of } \theta \text{ given } \mathscr{D}}{\textbf{Marginal likelihood}\ \text{or evidence}}$$

likelihood averaged over all potential θ

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$\div$

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- Maximum likelihood (ML/MLE), $\operatorname{argmax}_\theta\ p(\mathscr{D} \mid \theta)$ is equiv. empirical loss minimisation (ERM)
- Maximum a-posteriori (MAP), $\operatorname{argmax}_\theta\ p(\mathscr{D} \mid \theta) p(\theta)$ is equiv. regularised ERM
- Exact/approximate Bayesian inference

Linear regression - maximum likelihood

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Factorise across data points

Mean = linear mapping

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Maximum likelihood, $\operatorname{argmax}_\theta \, p(\mathcal{D} \mid \theta)$ **is equiv. to least squares**

Linear regression - Maximum a posteriori

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Prior: $p(\theta) = \mathcal{N}(\theta; \mathbf{0}, \sigma_o^2 \mathrm{I}) = \prod_d \mathcal{N}(\theta_d; 0, \sigma_o^2)$

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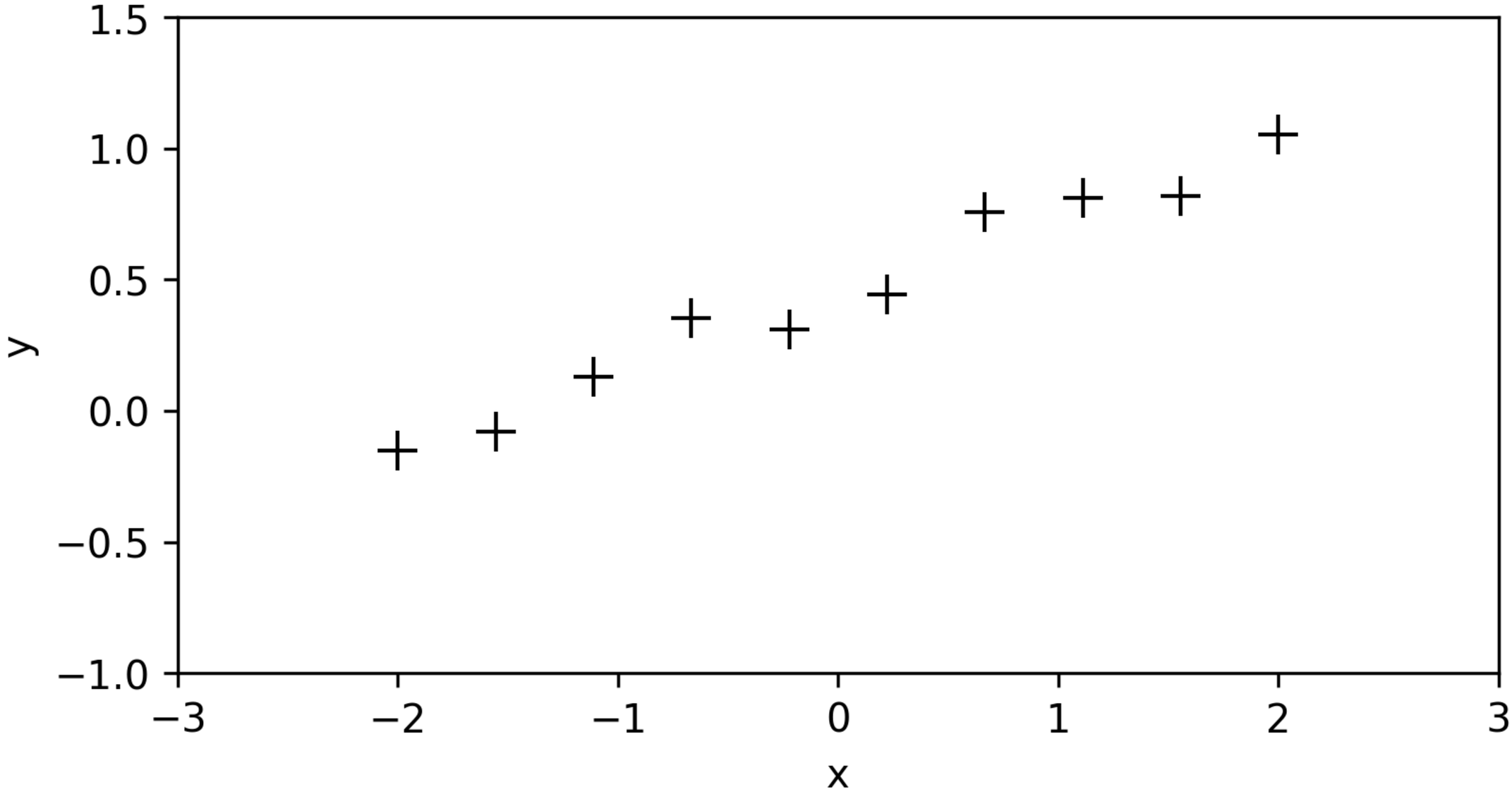

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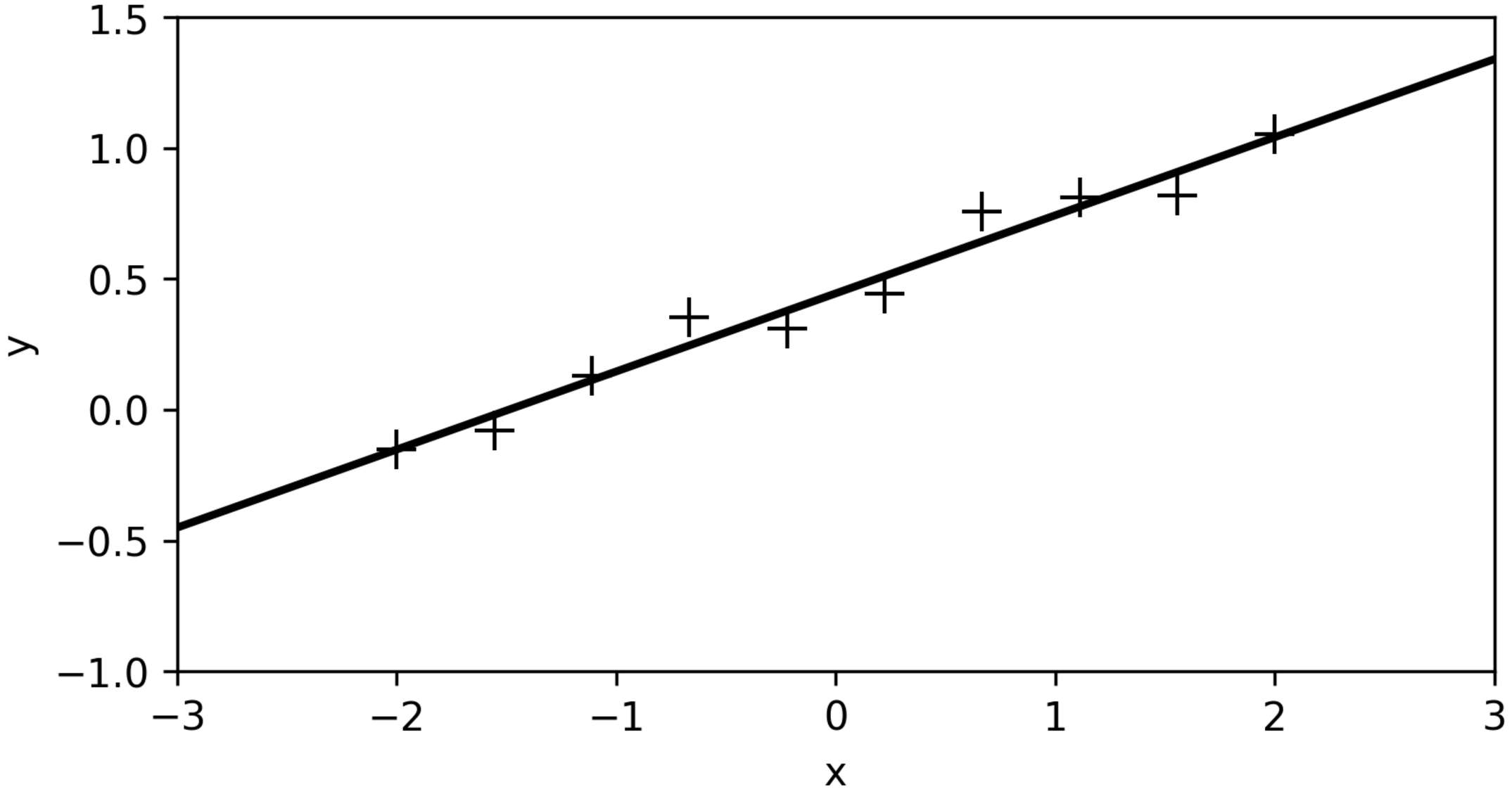

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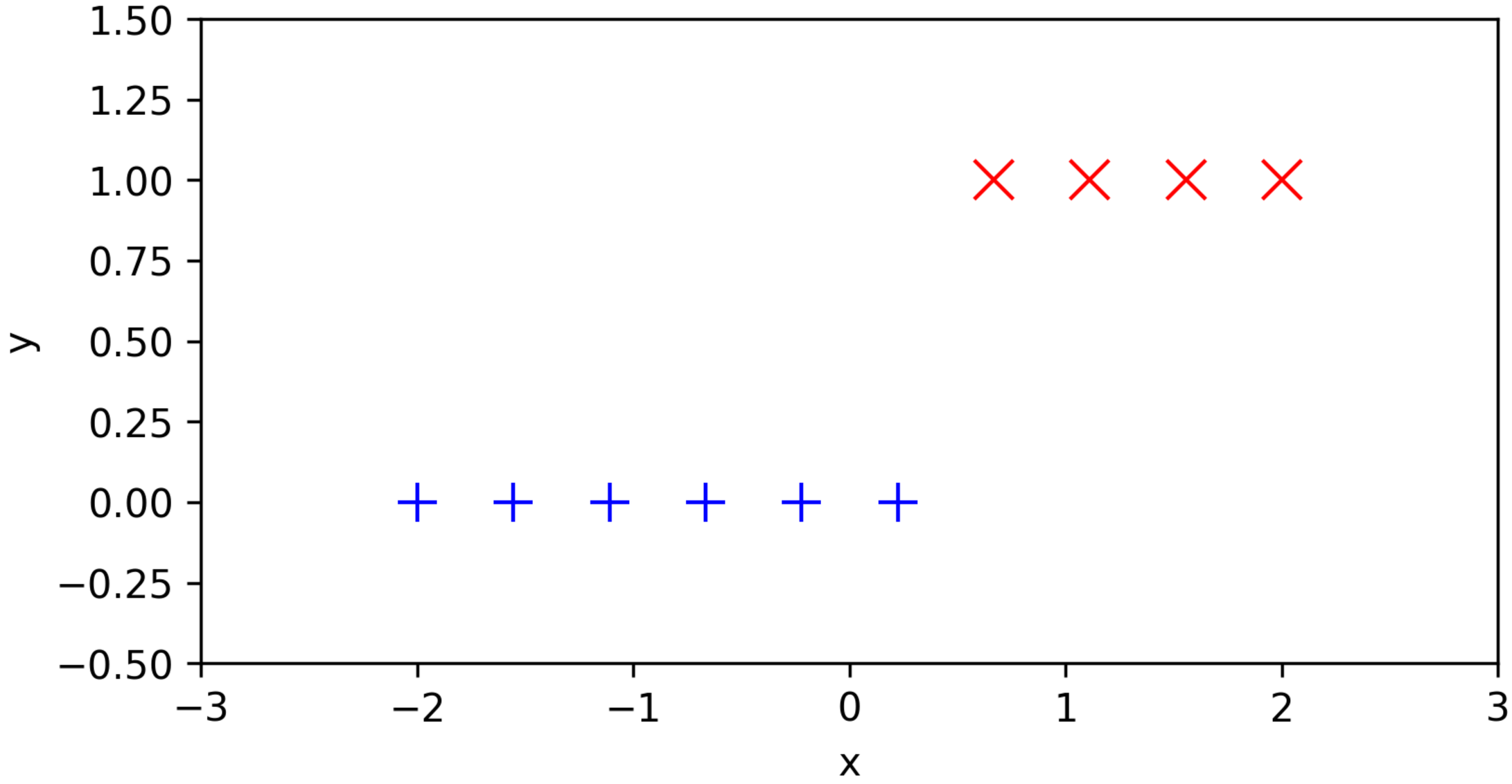

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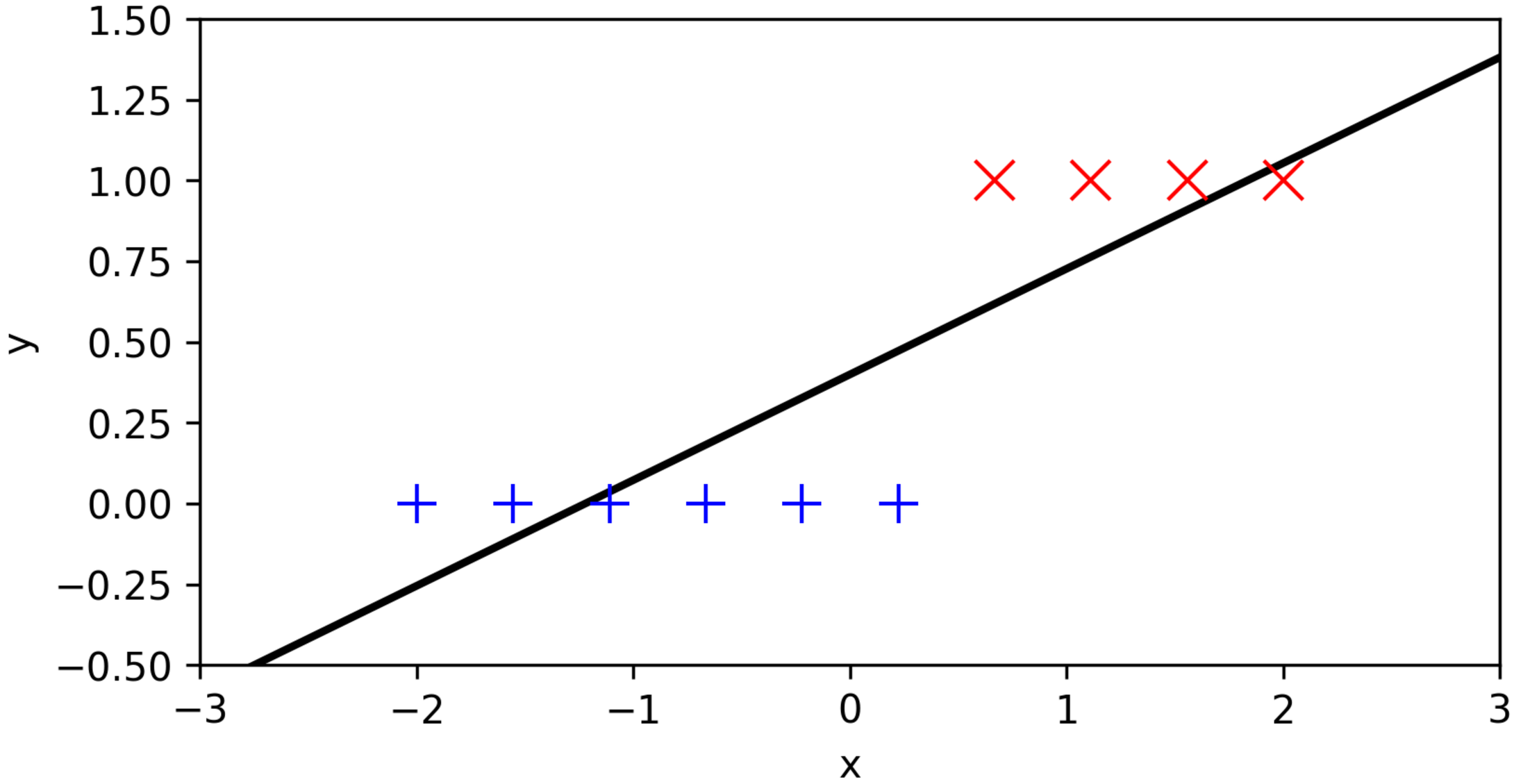

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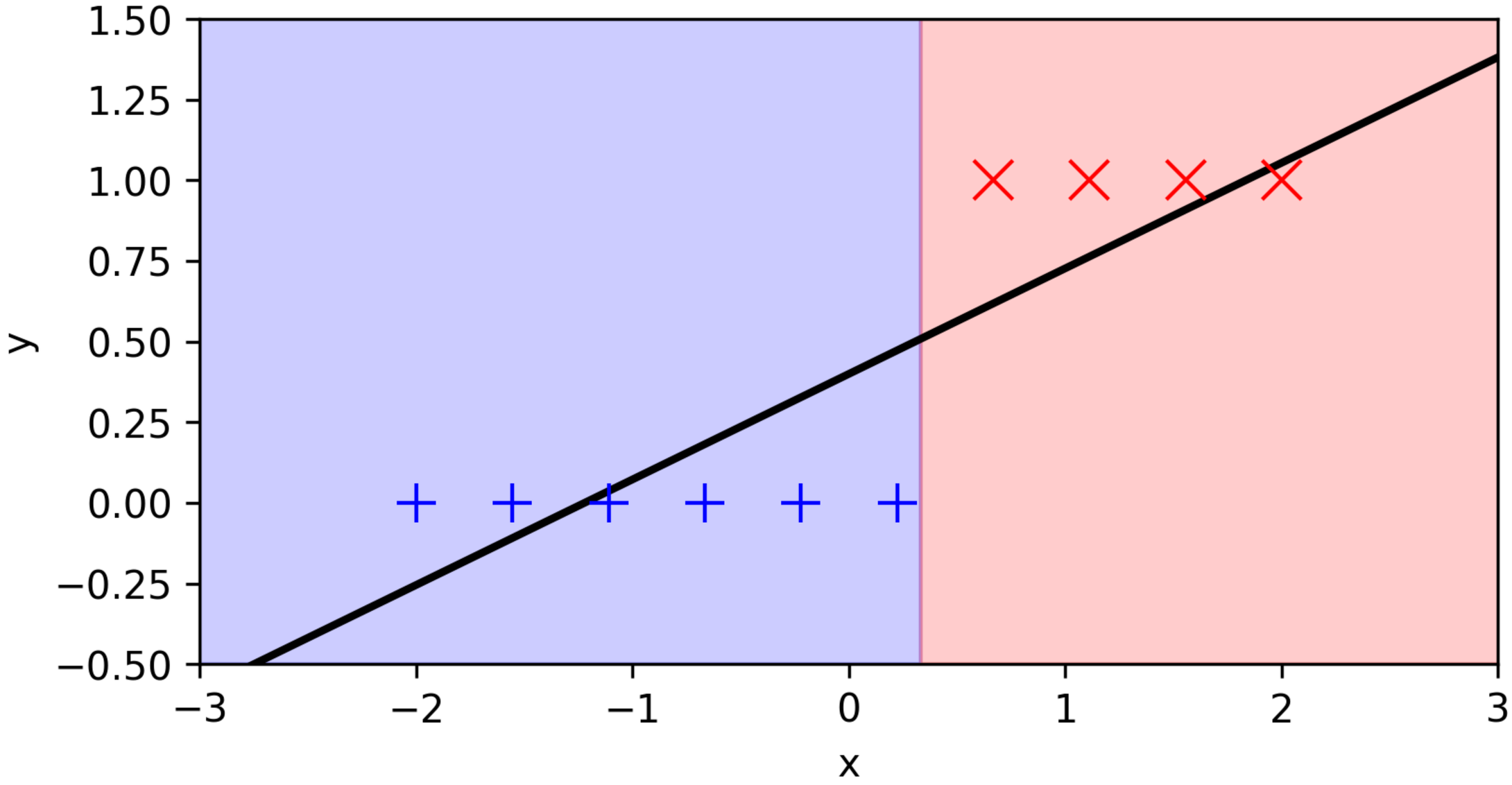

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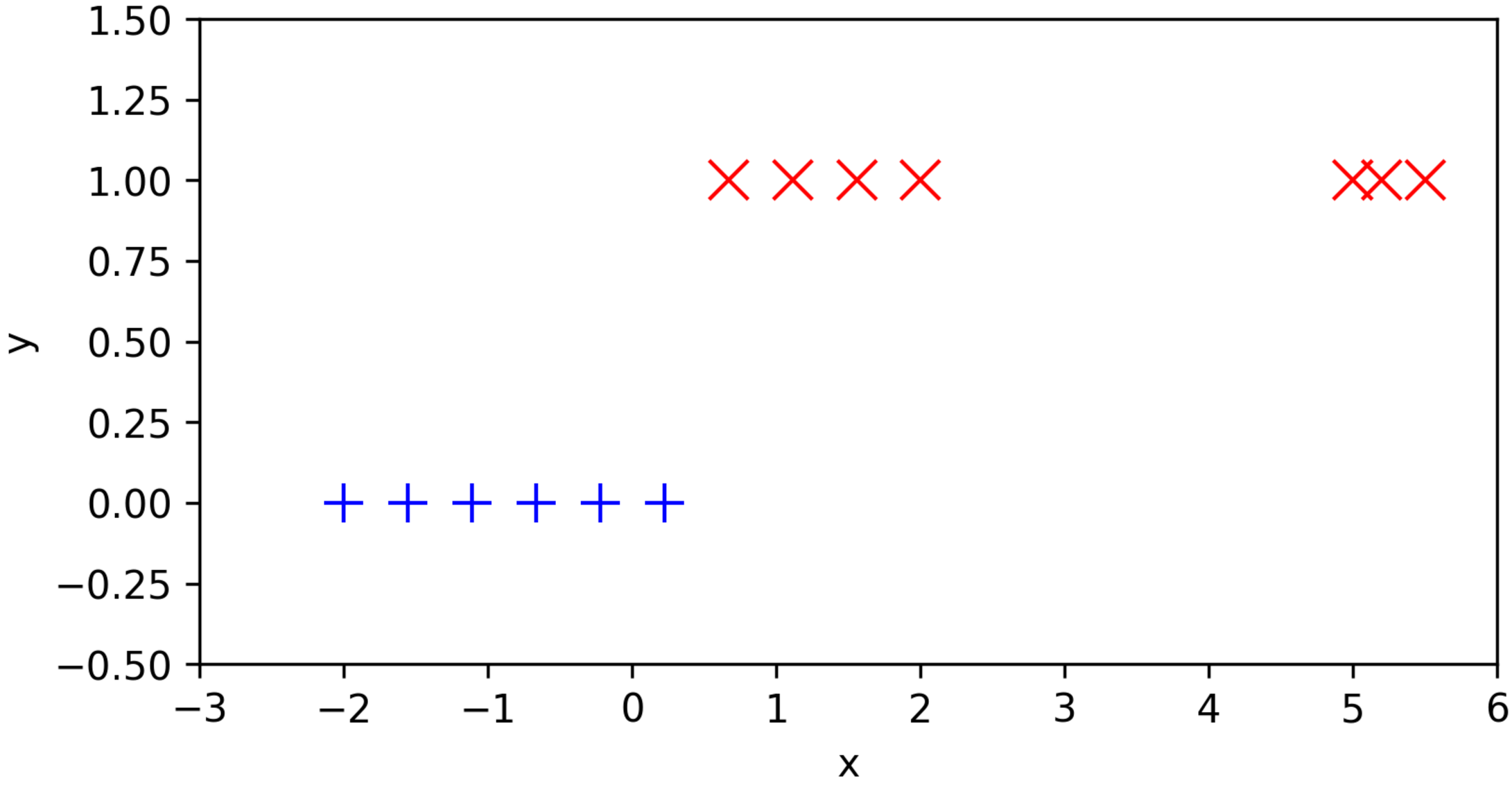

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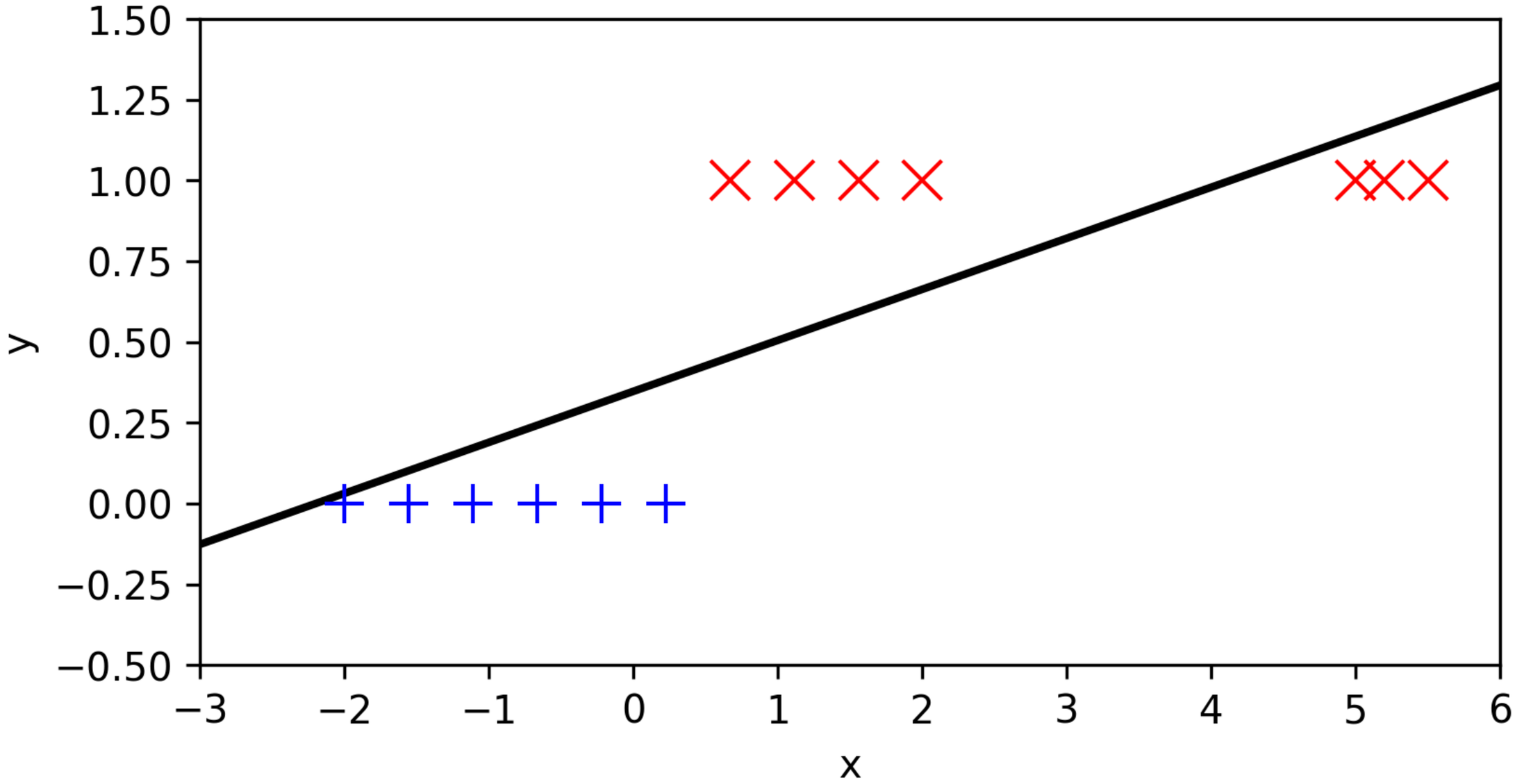

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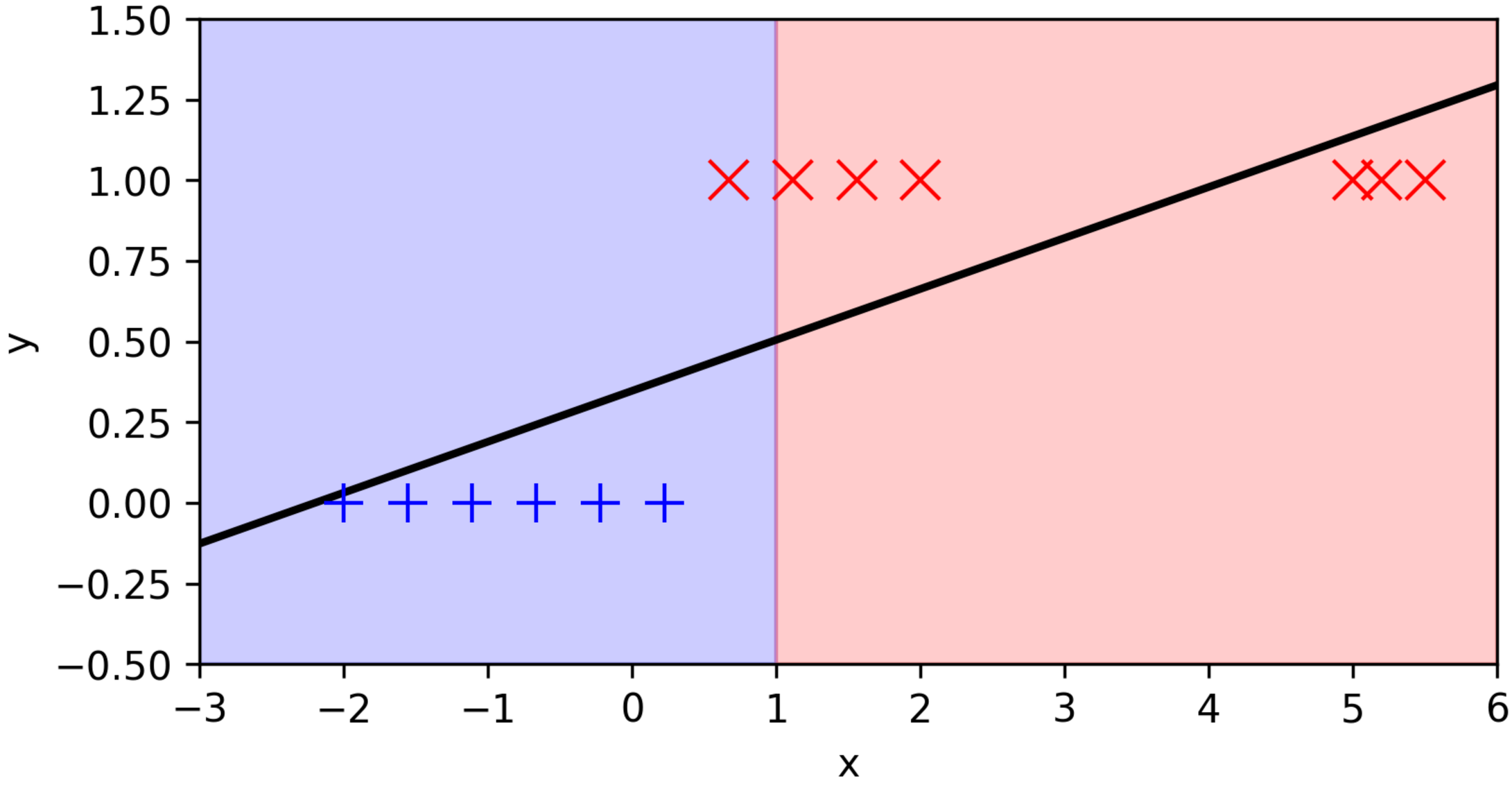
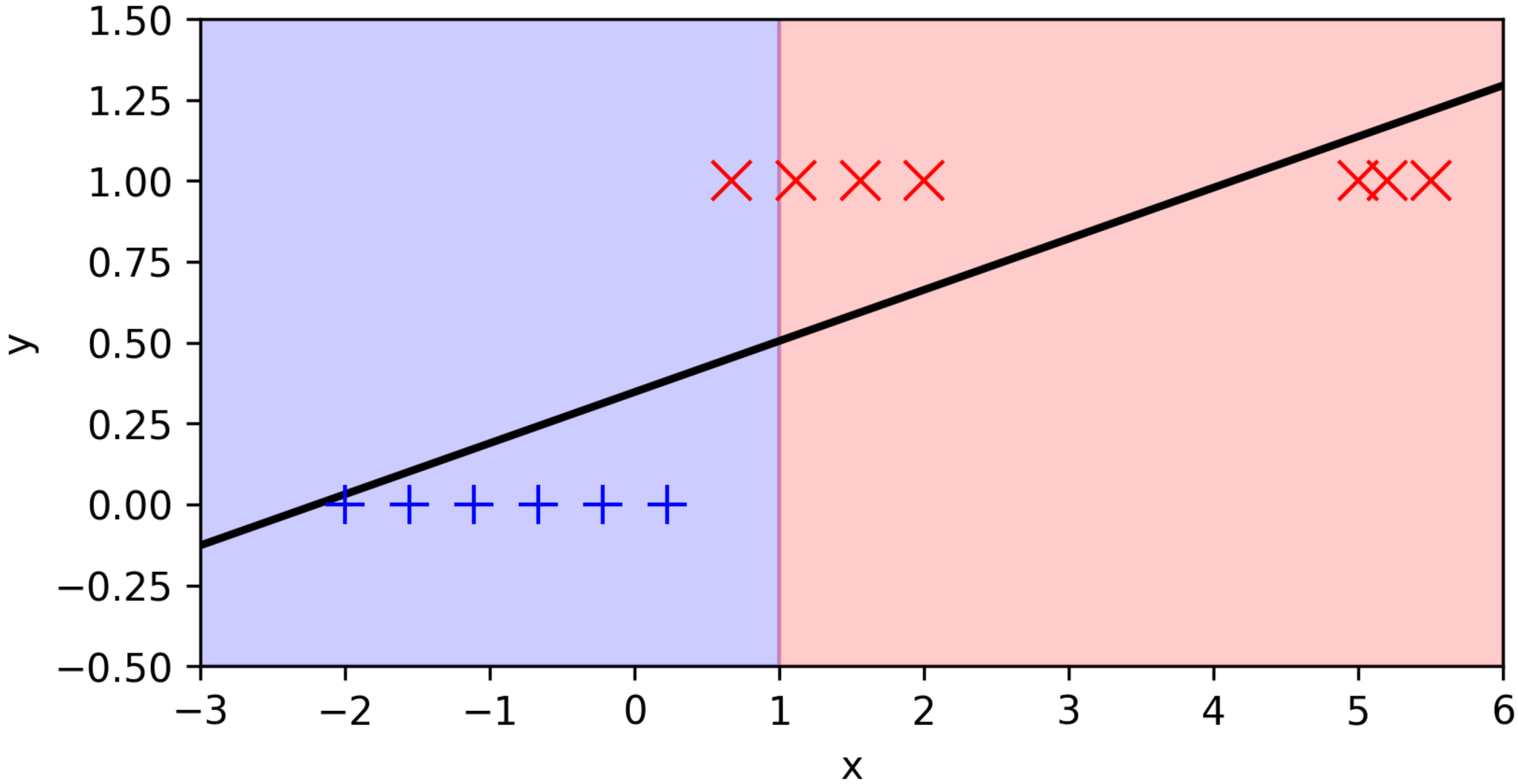


Can we use least squares to do binary classification? One more example



Least squares for classification: Lack robustness. Also fundamentally unsound - remember the Gaussian assumption!

Binary logistic classification - problem set-up

Binary logistic classification - problem set-up

Training data N input, output pairs $\mathscr{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}, \mathbf{x}_n \in \mathbb{R}^D,\ y_n \in \{0,1\}$

Each row is a data

Each column is a feature

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

One value per data point
0 or 1

Binary logistic classification - problem set-up

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Imagine: $p(y = 1 \,|\, x) = g_\theta(x)$ then $p(y = 0 \,|\, x) = 1 - g_\theta(x)$. **Constraint**: $0 \leq g_\theta(x) \leq 1, \forall x$

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Prediction with threshold = 0.5: $y = 1$ if $g_\theta(x) \geq 0.5$ and $y = 0$ if $g_\theta(x) < 0.5$.

Binary logistic classification - logistic function

Binary logistic classification - logistic function

Reminder: Linear regression: $f_\theta(\mathbf{x}) = \sum_{d=1}^{D} \theta_d x_d = \theta^\intercal \mathbf{x}, \theta \in \mathbb{R}^D$

$$\begin{bmatrix} f_\theta(\mathbf{x}_1) \\ f_\theta(\mathbf{x}_2) \\ \vdots \\ f_\theta(\mathbf{x}_N) \end{bmatrix} = \begin{bmatrix} \theta^\intercal \mathbf{x}_1 \\ \theta^\intercal \mathbf{x}_2 \\ \vdots \\ \theta^\intercal \mathbf{x}_N \end{bmatrix} = X\theta$$

Binary logistic classification - logistic function

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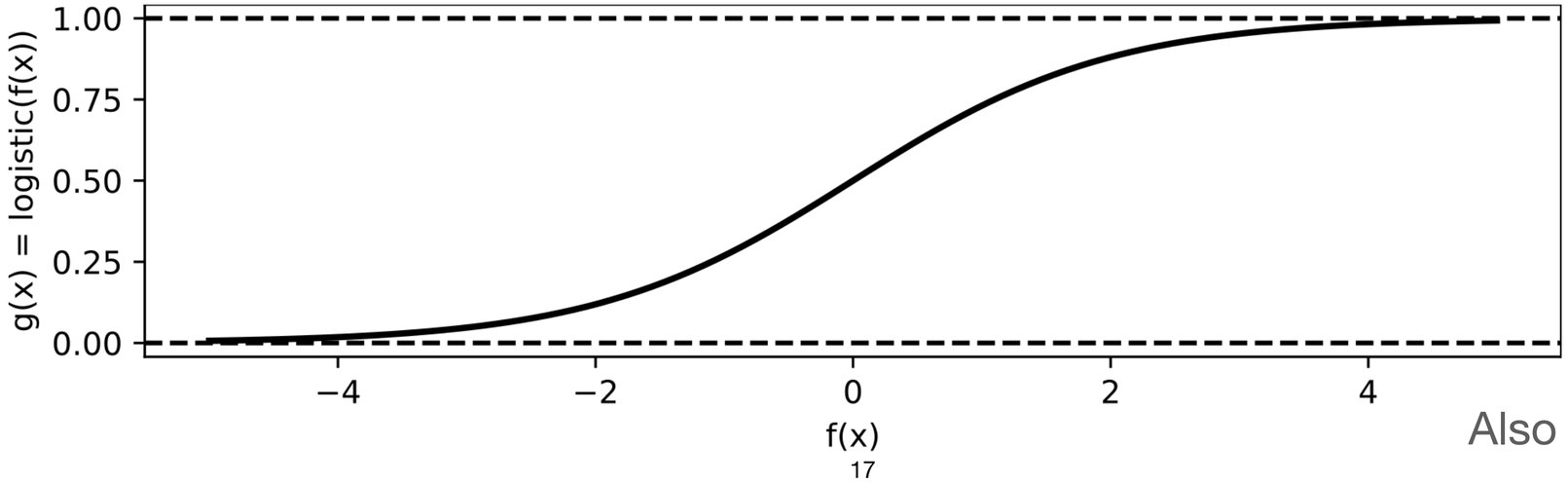
Want: $0 \leq g_\theta(x) \leq 1, \forall x$

Idea: 'squash' $f_\theta(x)$ through a *logistic sigmoid* function $g_\theta(x) = \sigma(f_\theta(x))$, where

$$\sigma(z) = \frac{\exp(z)}{1 + \exp(z)} = \frac{1}{1 + \exp(-z)}$$



Also called sigmoid

Binary logistic classification - maximum likelihood

Binary logistic classification - maximum likelihood

We can write down the ***likelihood*** of parameters given one data point:

$$p(y_n \,|\, x_n, \theta) = \begin{cases} g_\theta(x_n), & \text{if } y_n = 1 \\ 1 - g_\theta(x_n), & \text{if } y_n = 0 \end{cases}$$

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We want to *maximise* the likelihood or *minimise* the negative log-likelihood:

$$\begin{aligned} \mathscr{L}_n(\theta) &= -\log p(y_n \,|\, x_n, \beta) = \begin{cases} -\log(g_\theta(x_n)), & \text{if } y_n = 1 \\ -\log(1 - g_\theta(x_n)), & \text{if } y_n = 0 \end{cases} \\ &= -y_n \log(g_\theta(x_n)) - (1 - y_n)\log(1 - g_\theta(x_n)) \end{aligned}$$

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For N datapoints:

$$\mathscr{L}(\theta) = \frac{1}{N} \sum_{n=1}^{N} -y_n \log(g_\theta(x_n)) - (1 - y_n)\log(1 - g_\theta(x_n))$$

Often called the **binary cross-entropy loss**

Binary logistic classification - gradients

Binary logistic classification - gradients

Objective: $\mathscr{L}(\theta) = \frac{1}{N}\sum_{n=1}^{N} -y_n \log(g_\theta(x_n)) - (1-y_n)\log(1-g_\theta(x_n))$

Notes: $g_\theta(x) = \sigma(f_\theta(x))$, σ is a logistic sigmoid, and $f_\theta(\mathbf{x}) = \sum_{d=1}^{D} \theta_d x_d = \theta^\intercal \mathbf{x}, \theta \in \mathbb{R}^D$

Show: $\frac{\mathrm{d}\mathscr{L}(\theta)}{\mathrm{d}\theta} = \frac{1}{N}\sum_{n=1}^{N} (g_\theta(x_n) - y_n)x_n^T$

Binary logistic classification - optimisation

Binary logistic classification - optimisation

We can use *gradient descent [Week 7]* to optimise $\mathscr{L}(\theta)$.

(i) Have some random starting point for θ

(ii) Update θ to decrease the loss function $\mathscr{L}(\theta)$, $\theta \leftarrow \theta - \gamma \left[\frac{\mathrm{d}\mathscr{L}(\theta)}{\mathrm{d}\theta}\right]^{\mathsf{T}}$

(iii) Repeat (ii) until reaching a minimum (convergence) [global minimum for logistic reg]

Regularised logistic classification

Similar to least squares, we want to *penalise* the amplitude of parameters by **regularisation:**

$$\mathscr{L}_\lambda(\theta) = \text{cross-entropy loss} + \lambda \|\theta\|_p^p$$

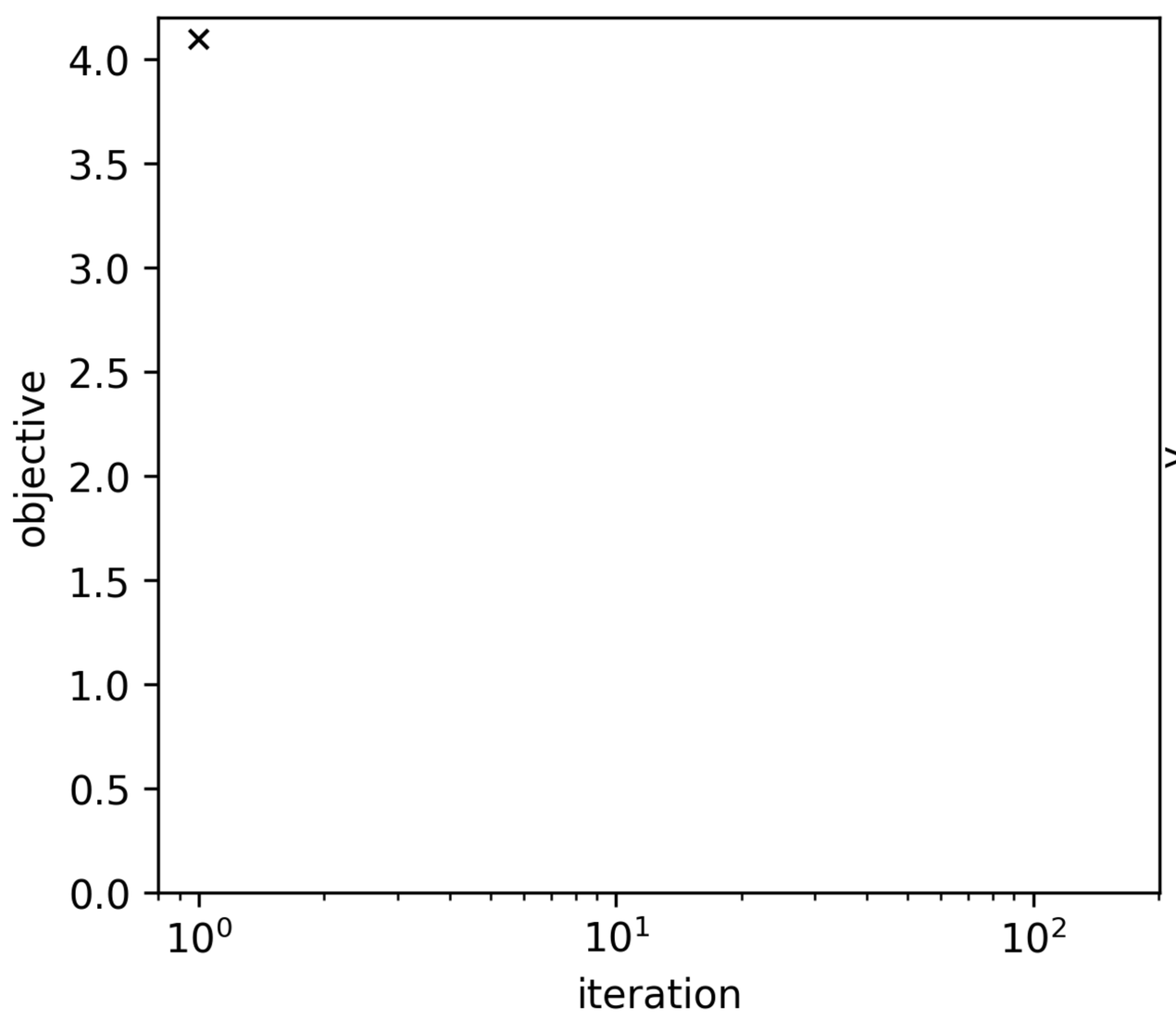
Data-fit
Lower = better fit

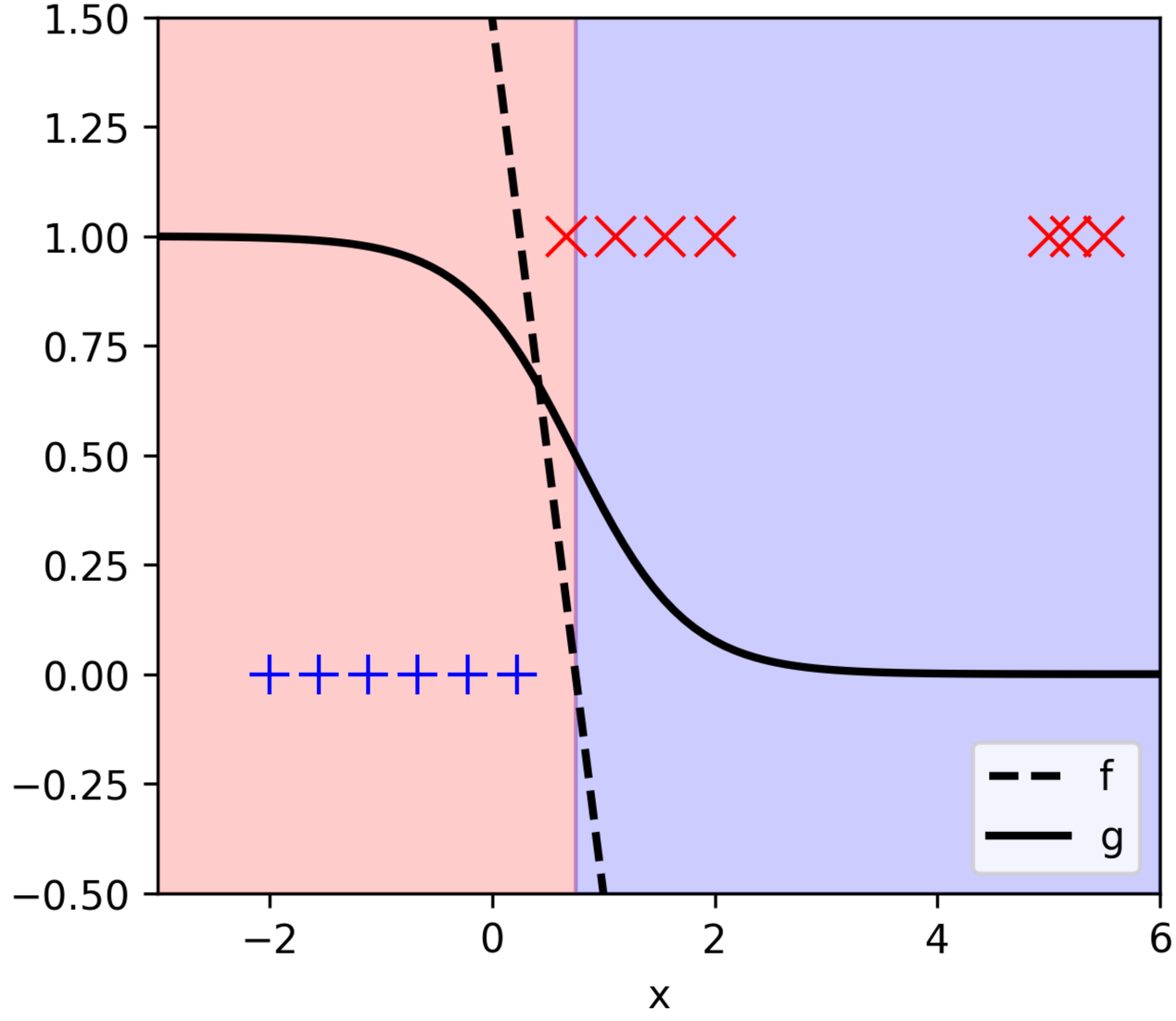
Regulariser
Lower = simpler model

Hyperparameter

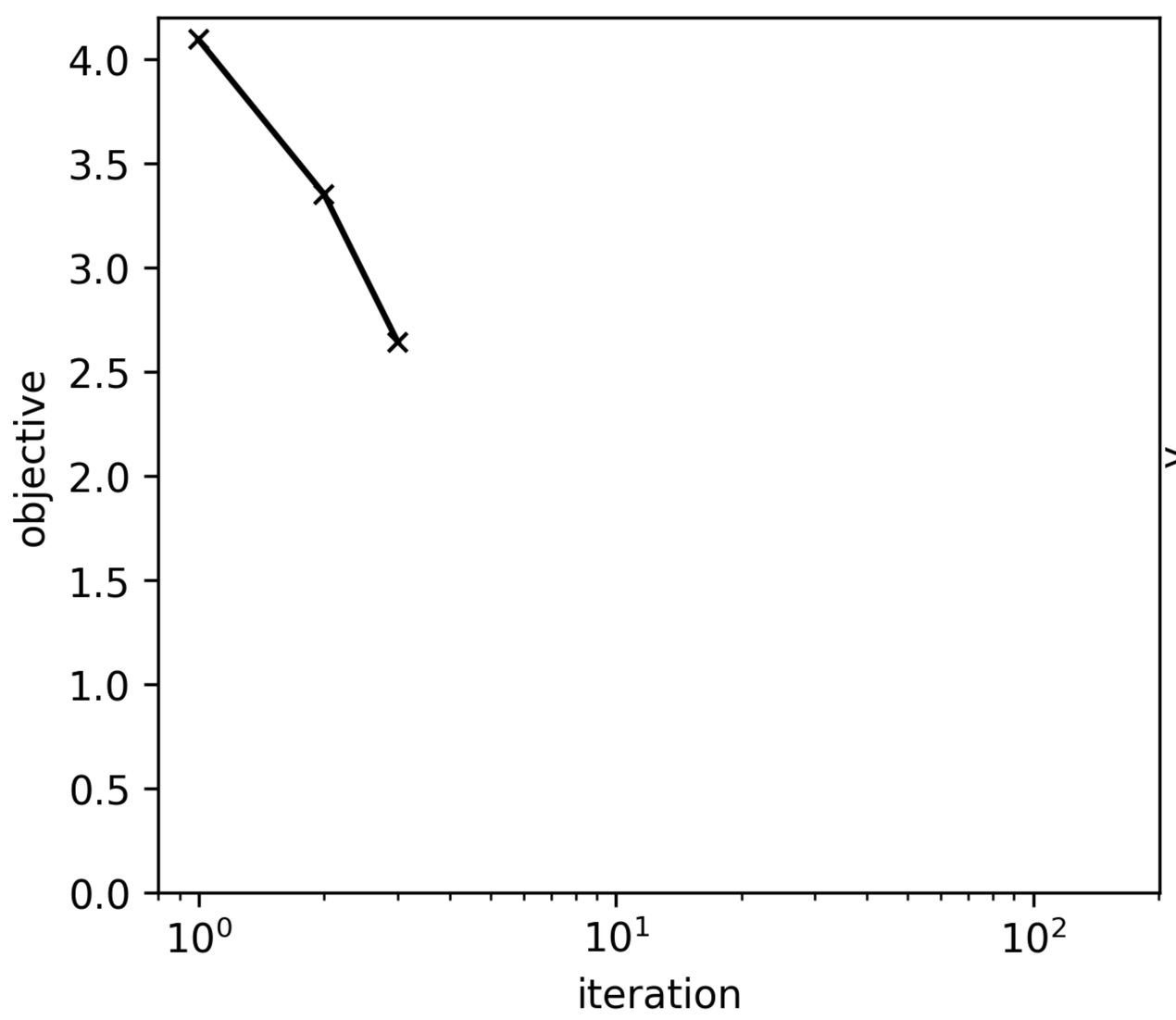
Binary logistic classification - example

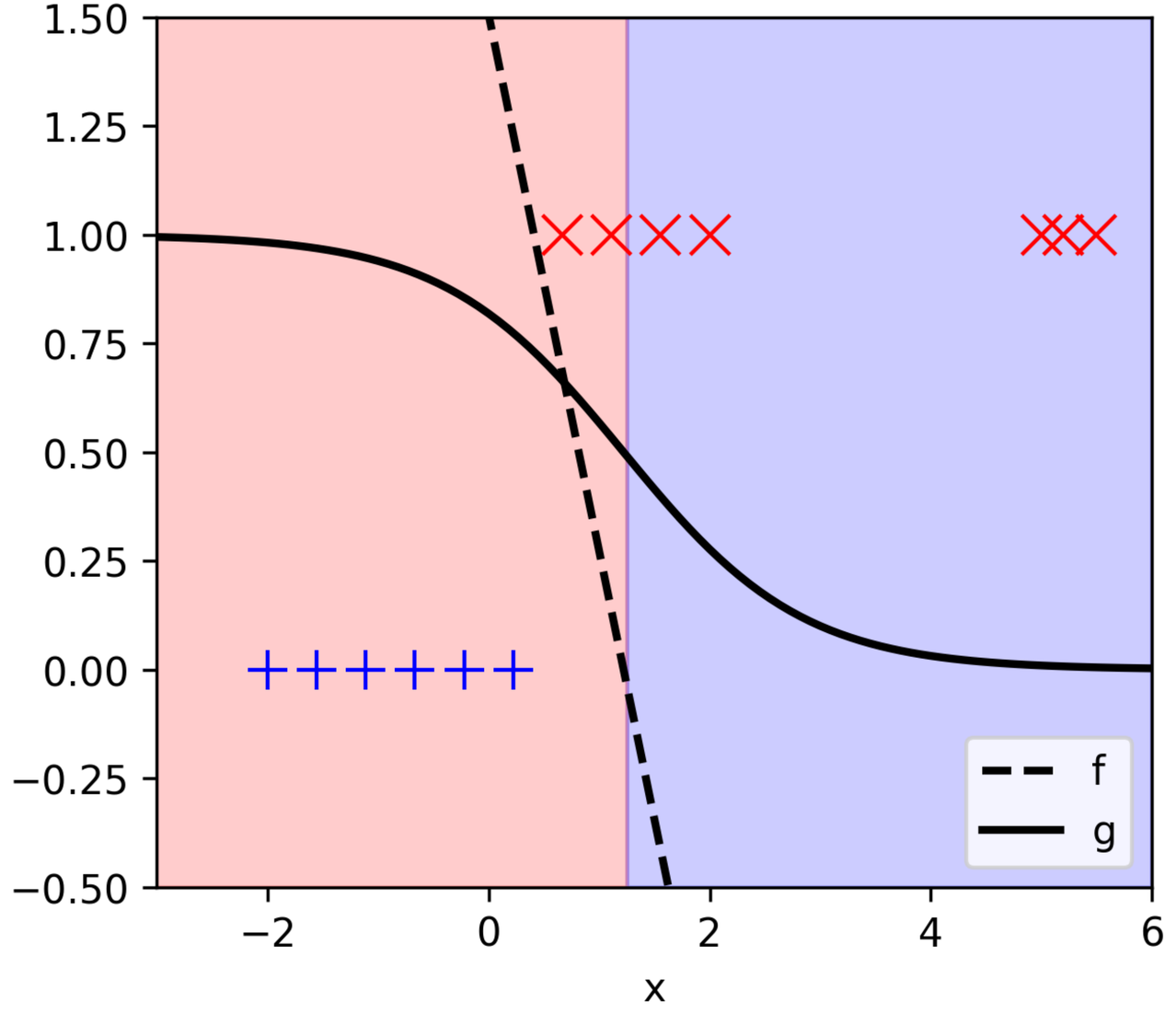
Binary logistic classification - example





Binary logistic classification - example





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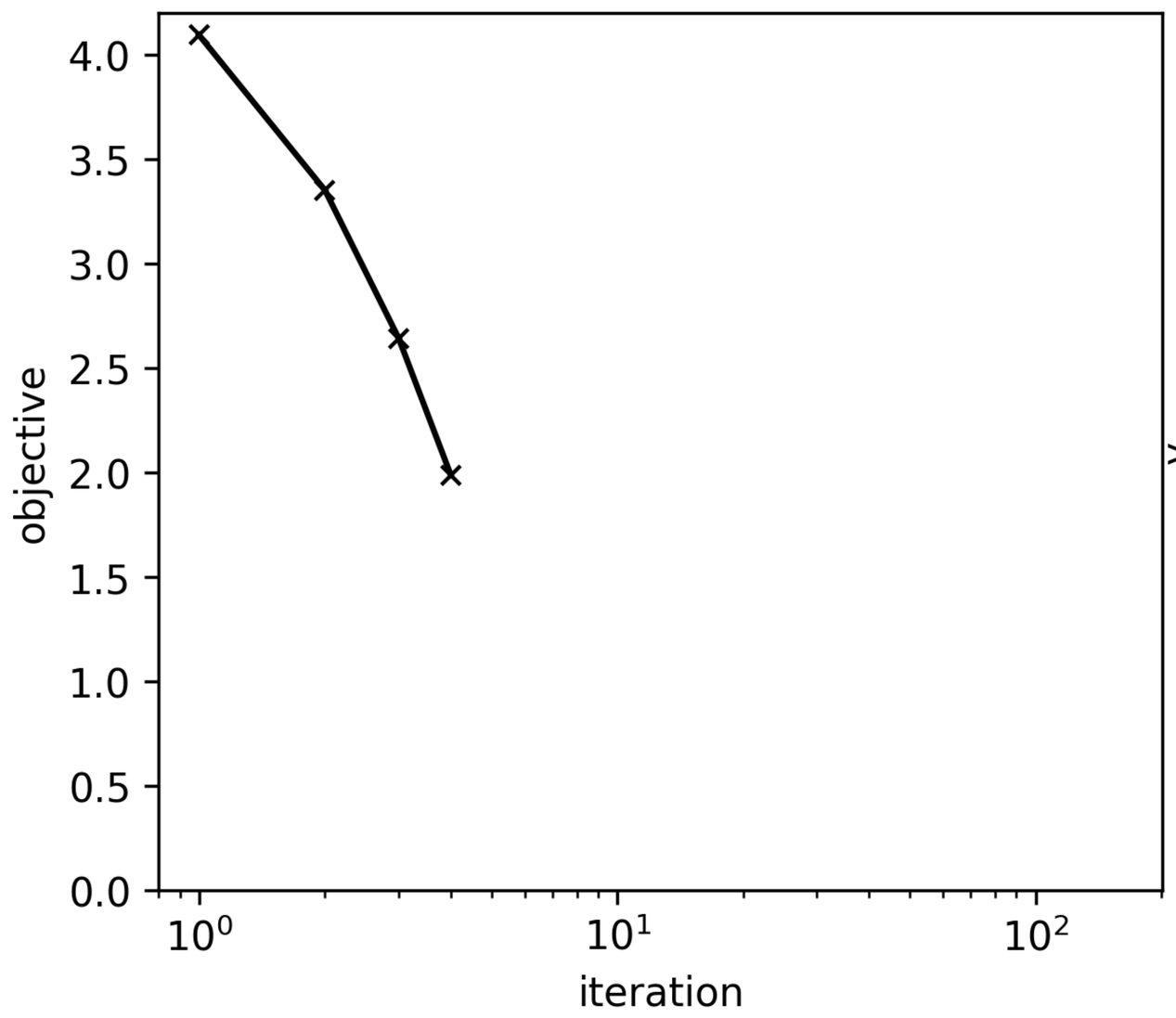

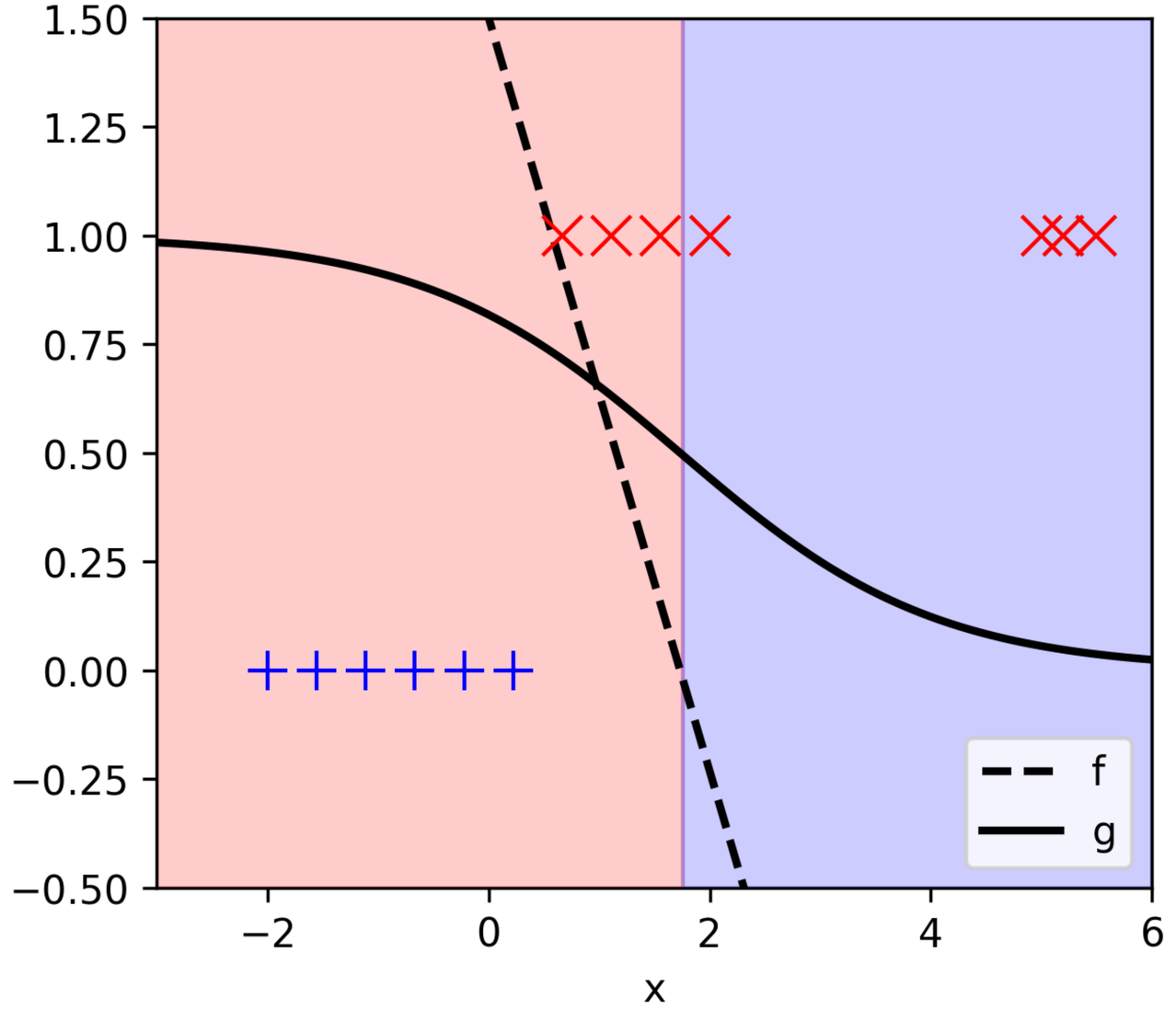

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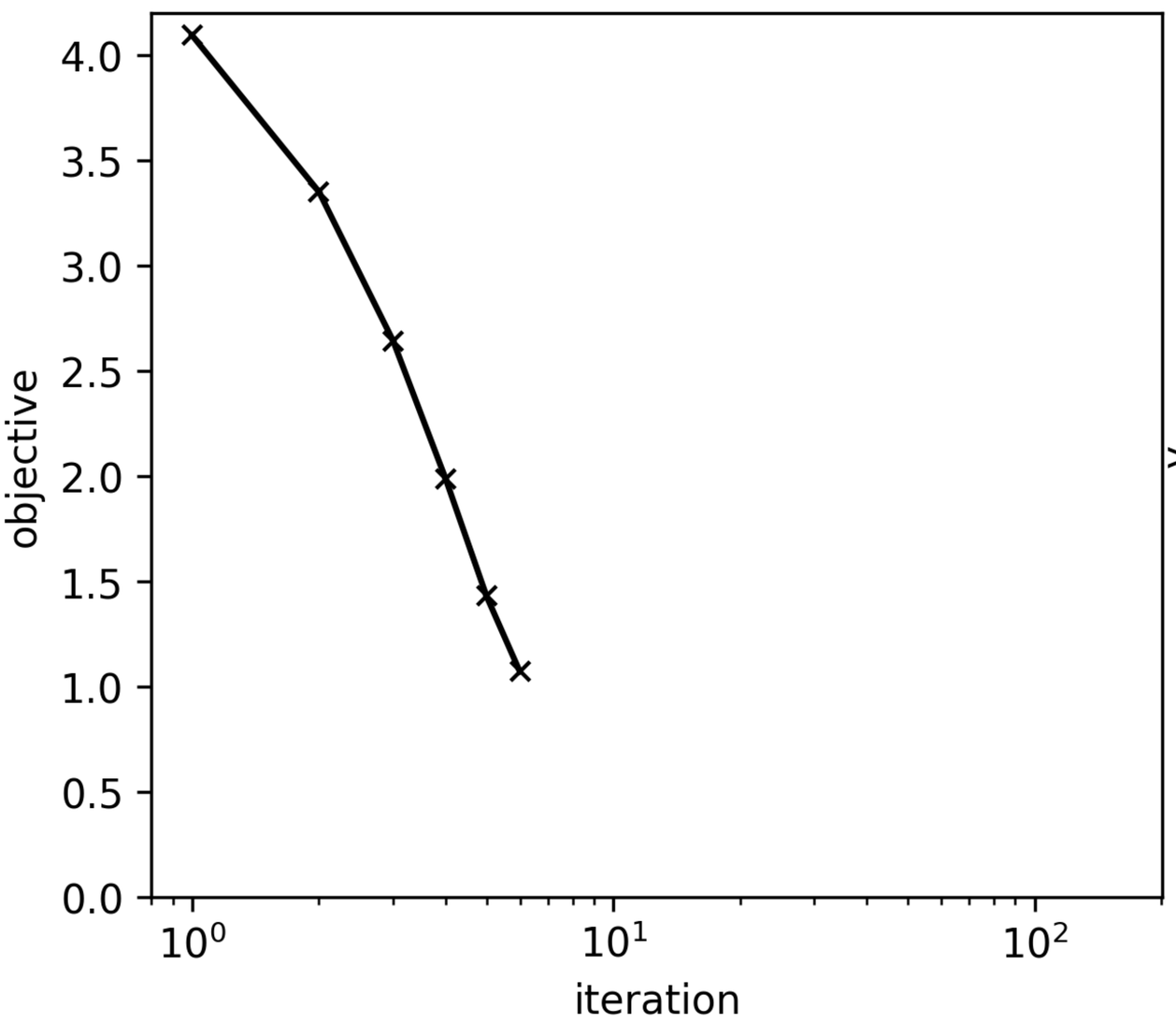

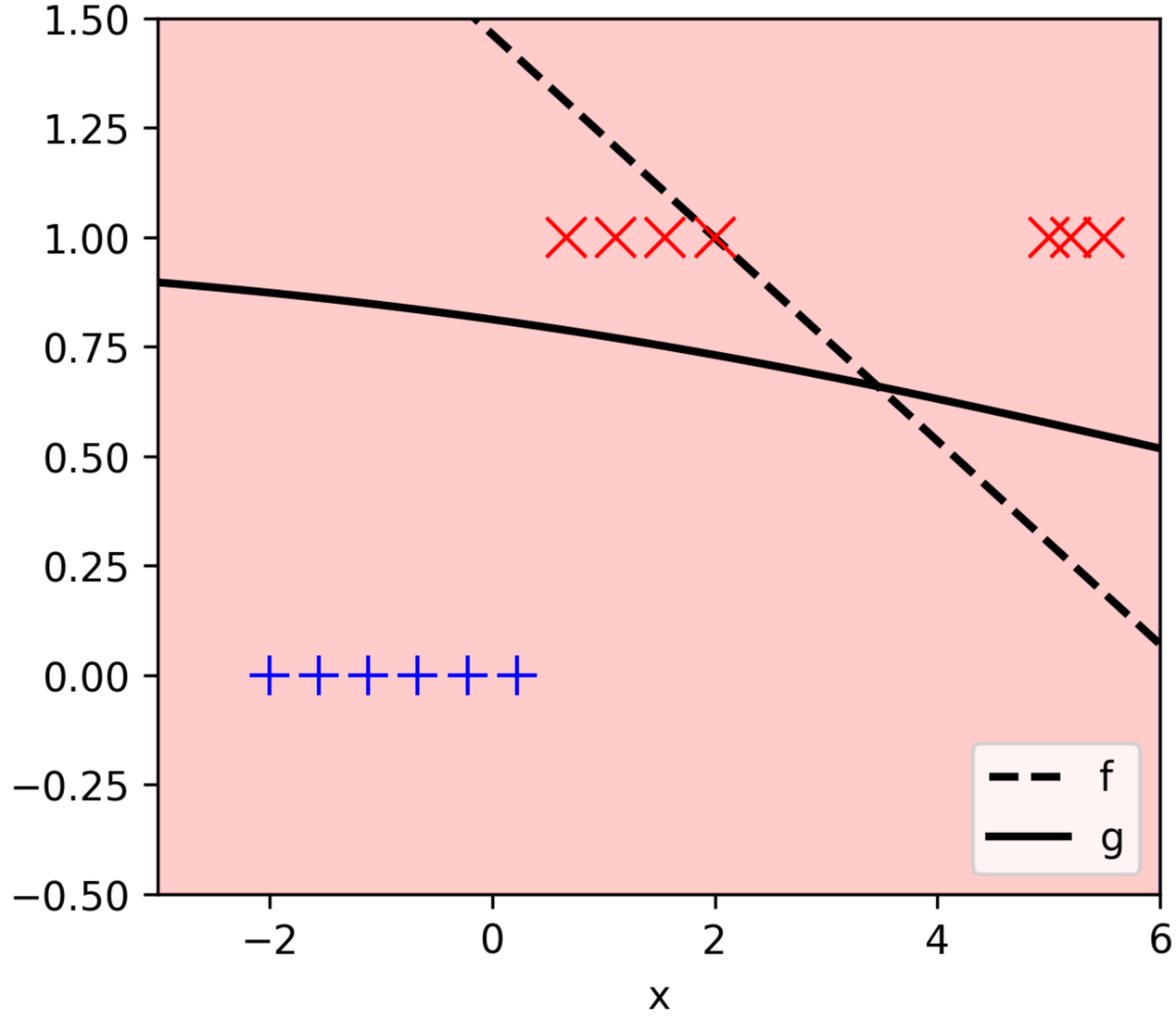

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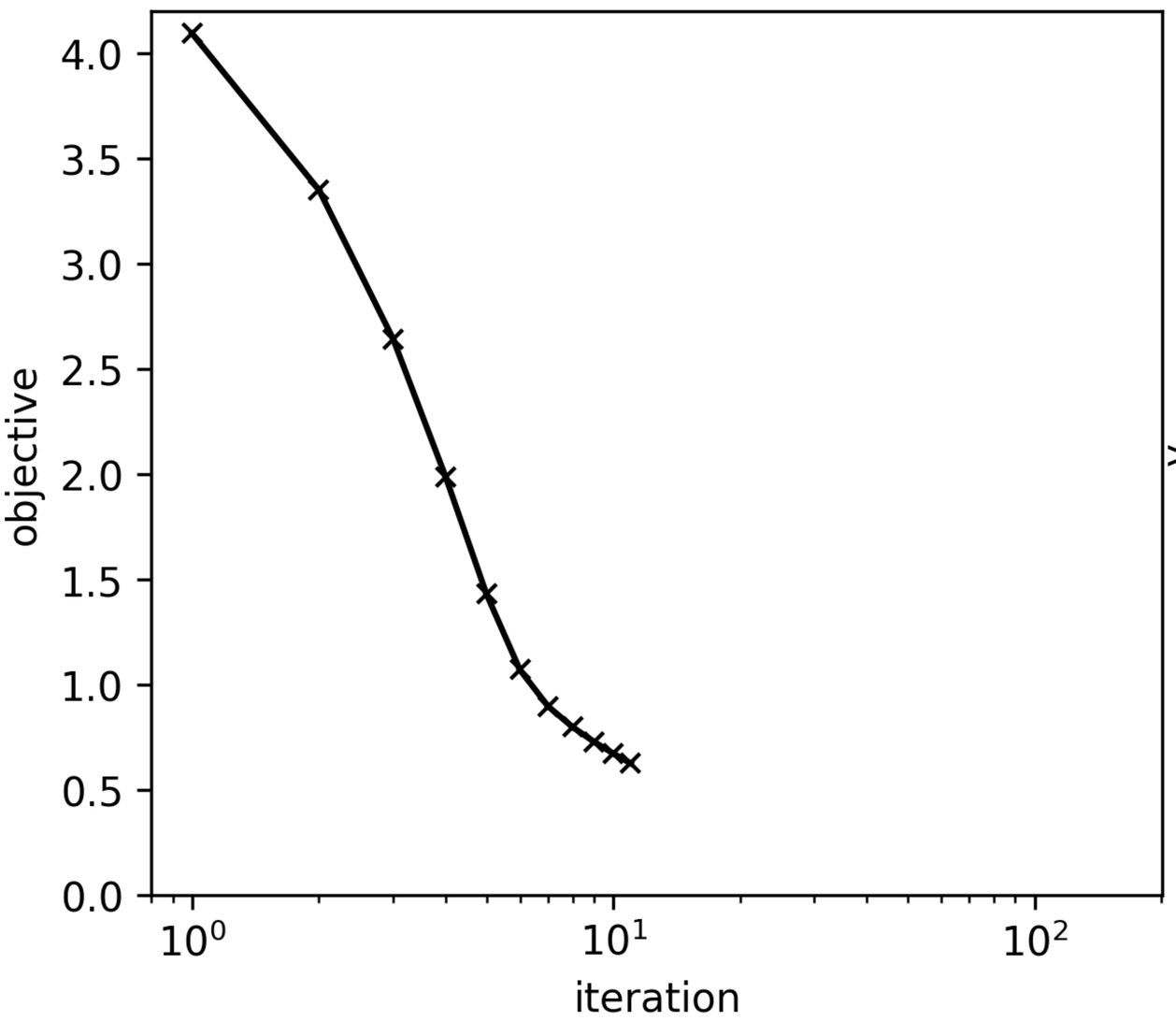

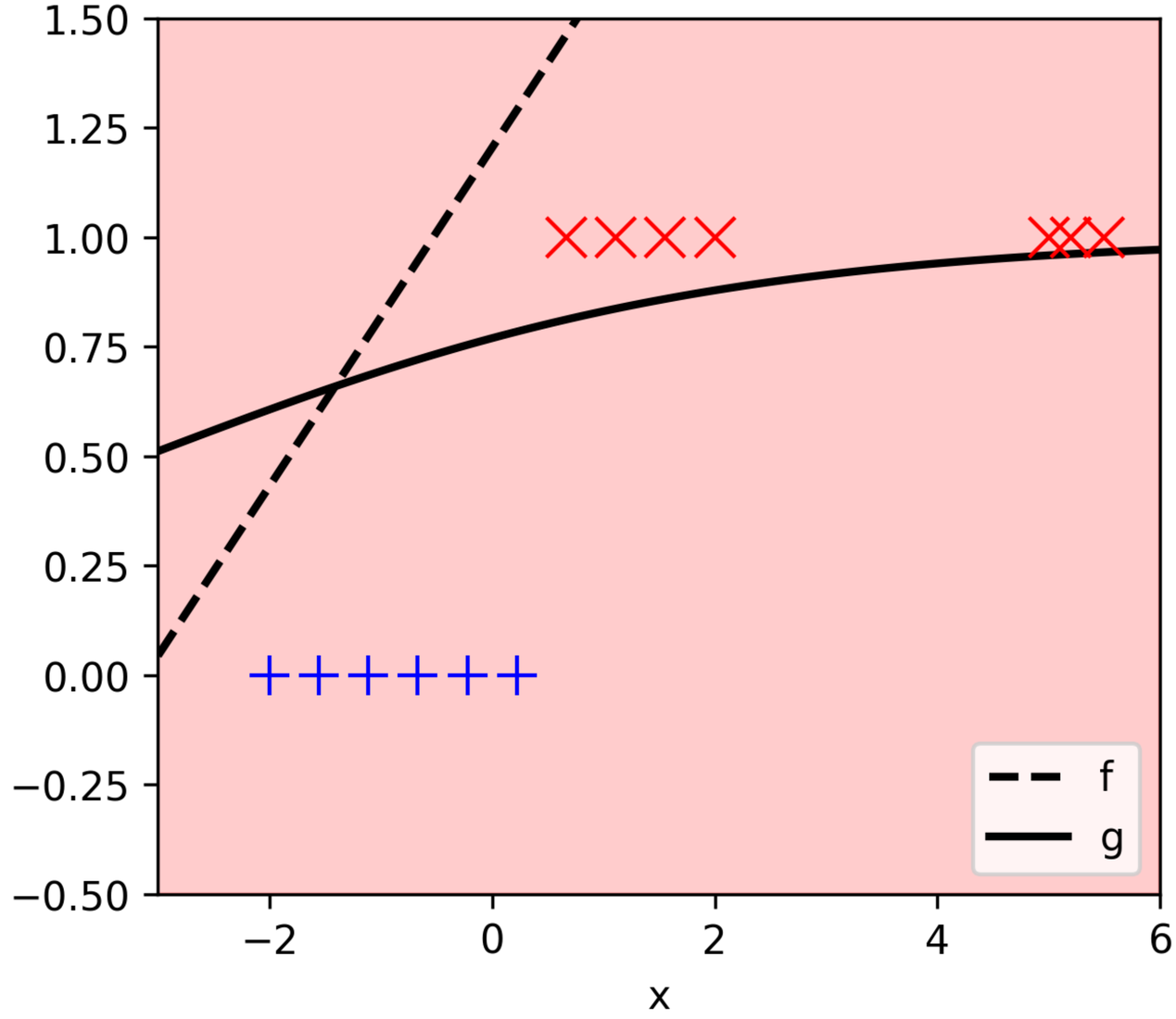

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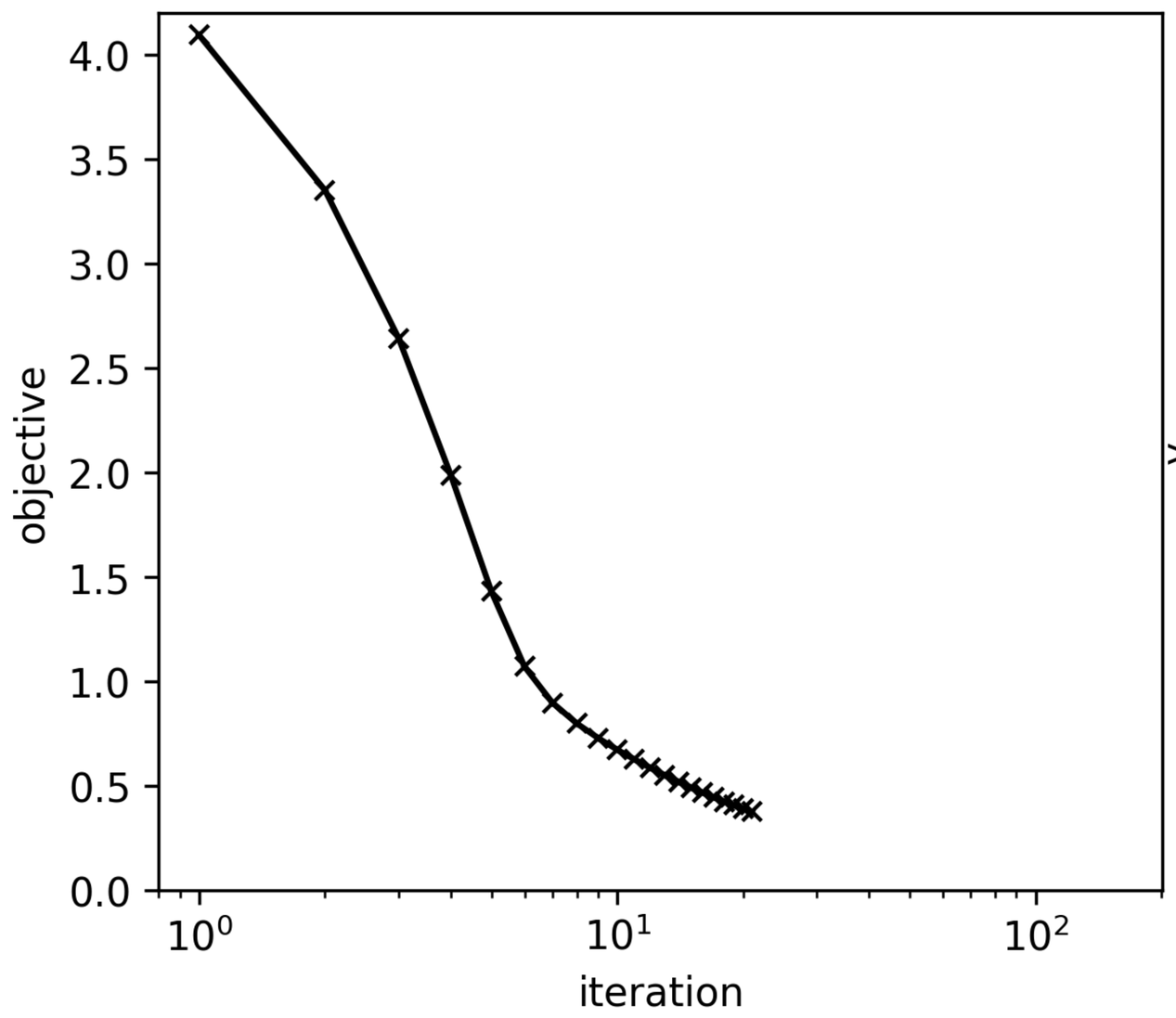

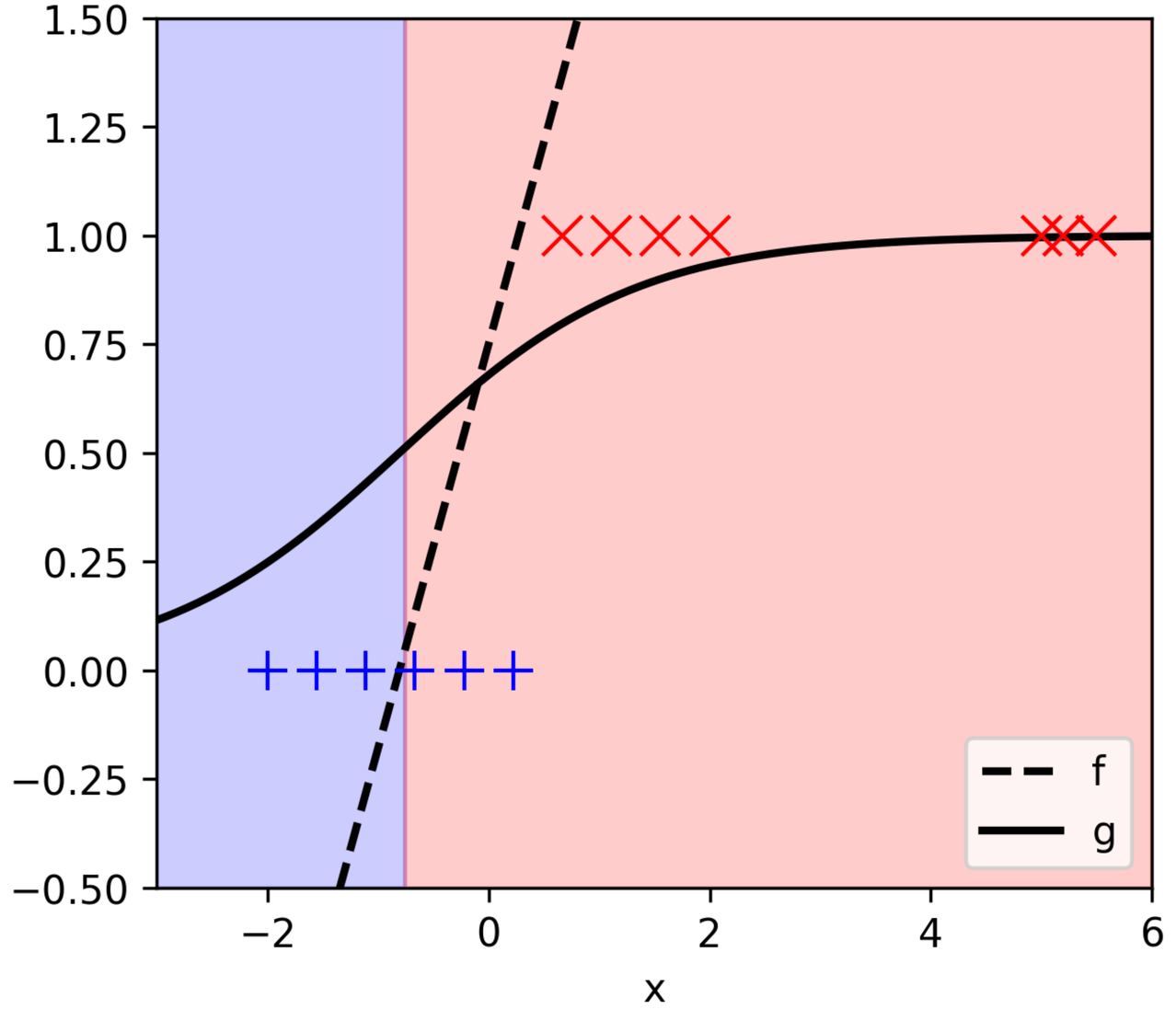

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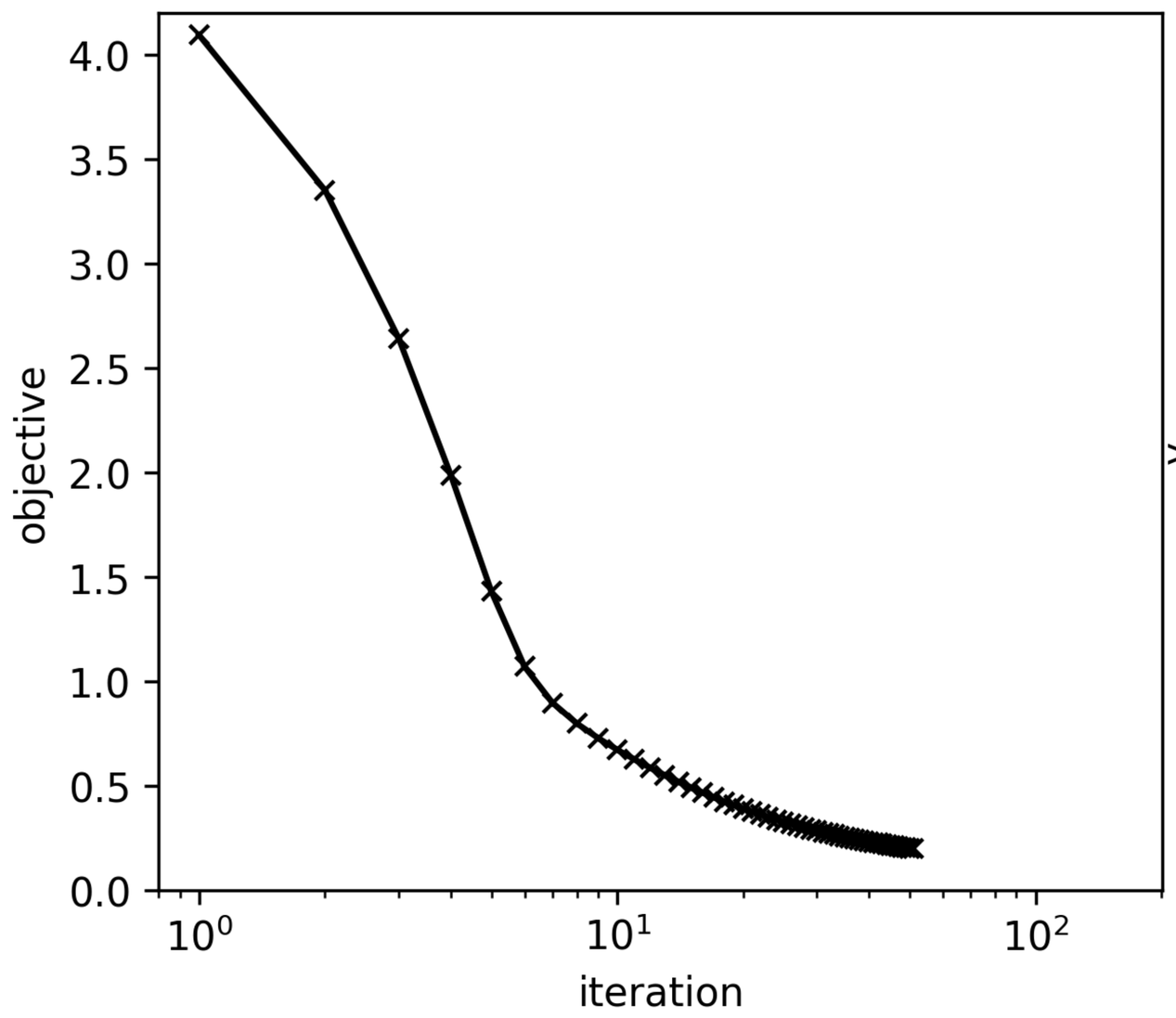

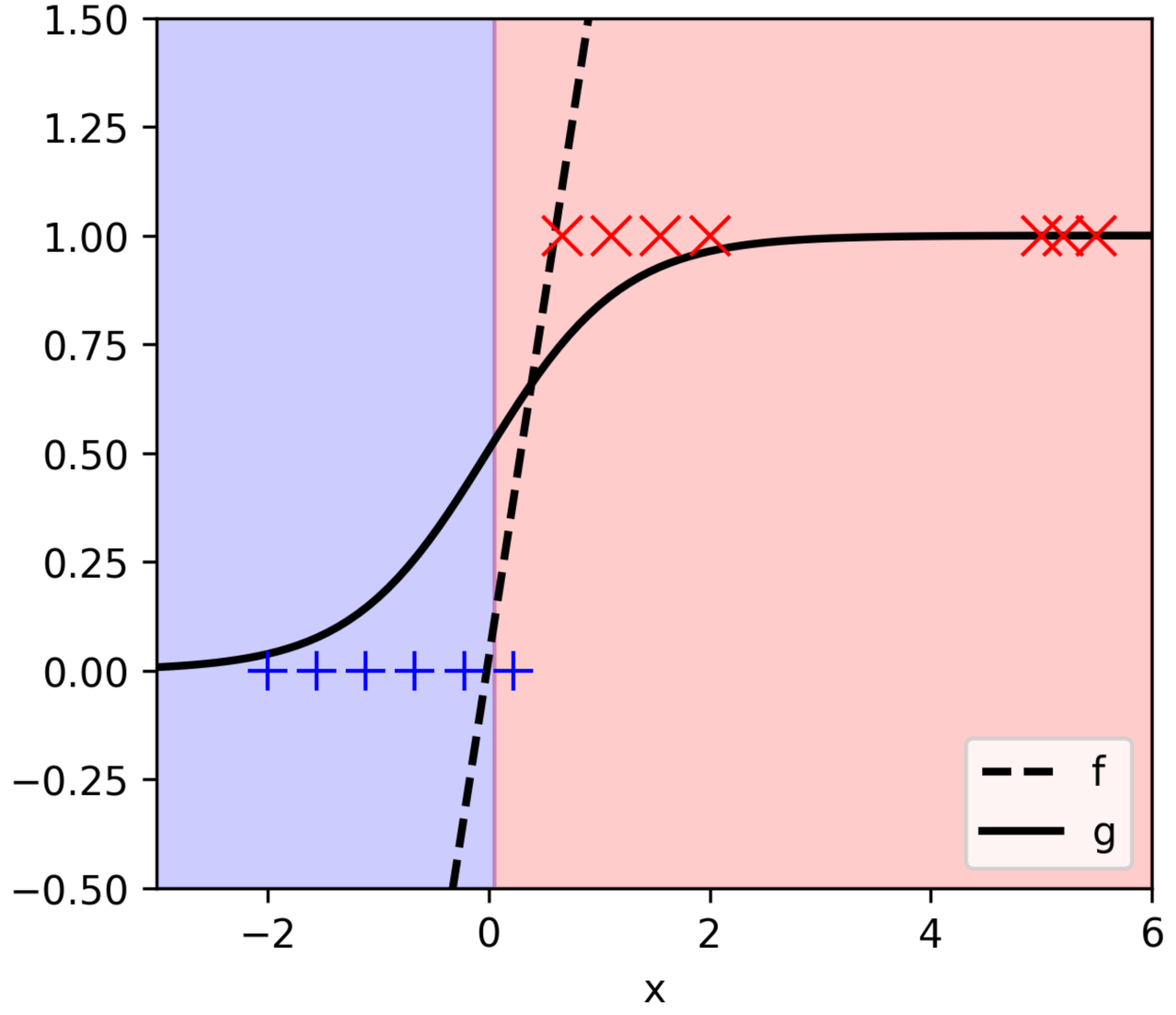

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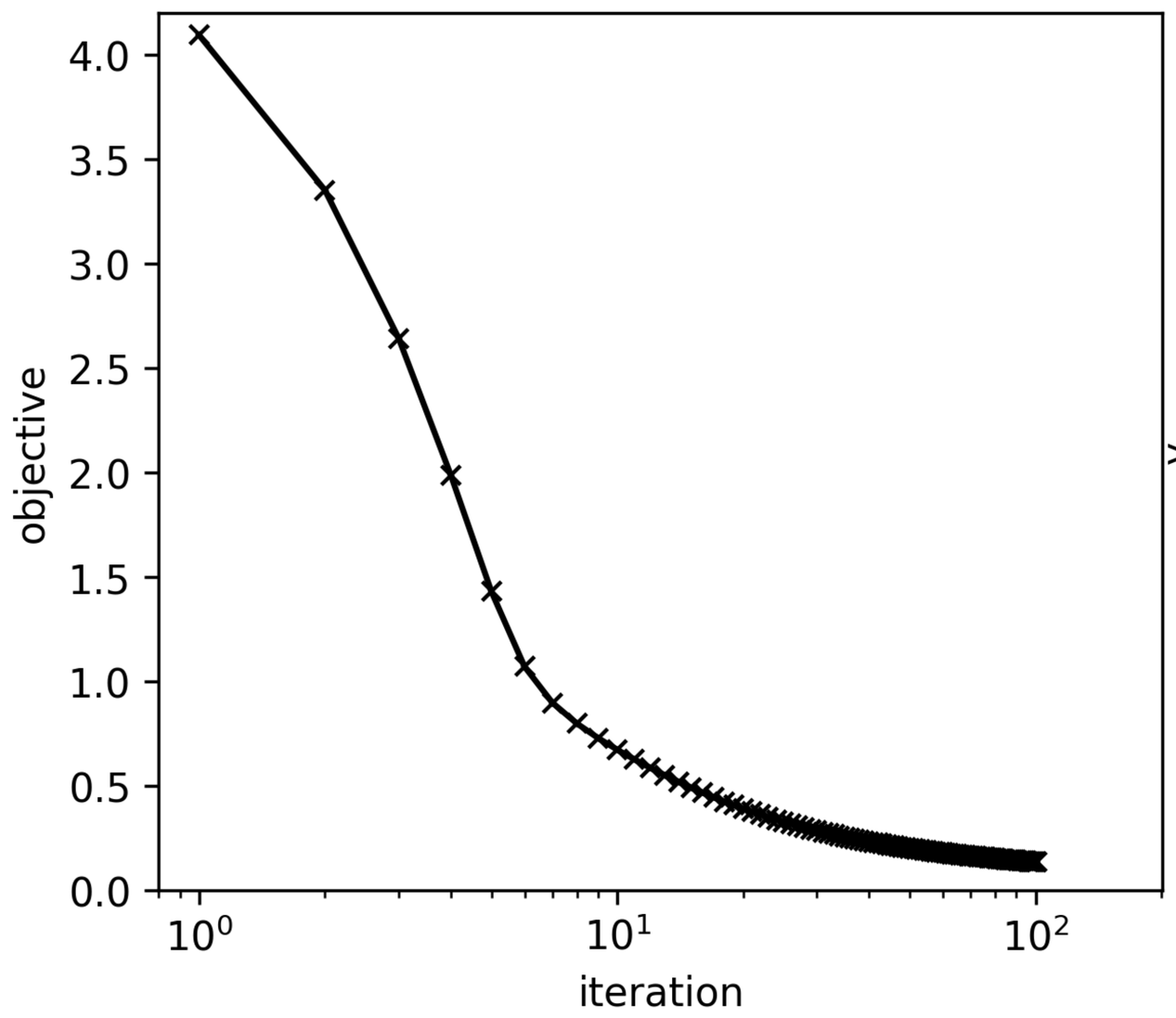

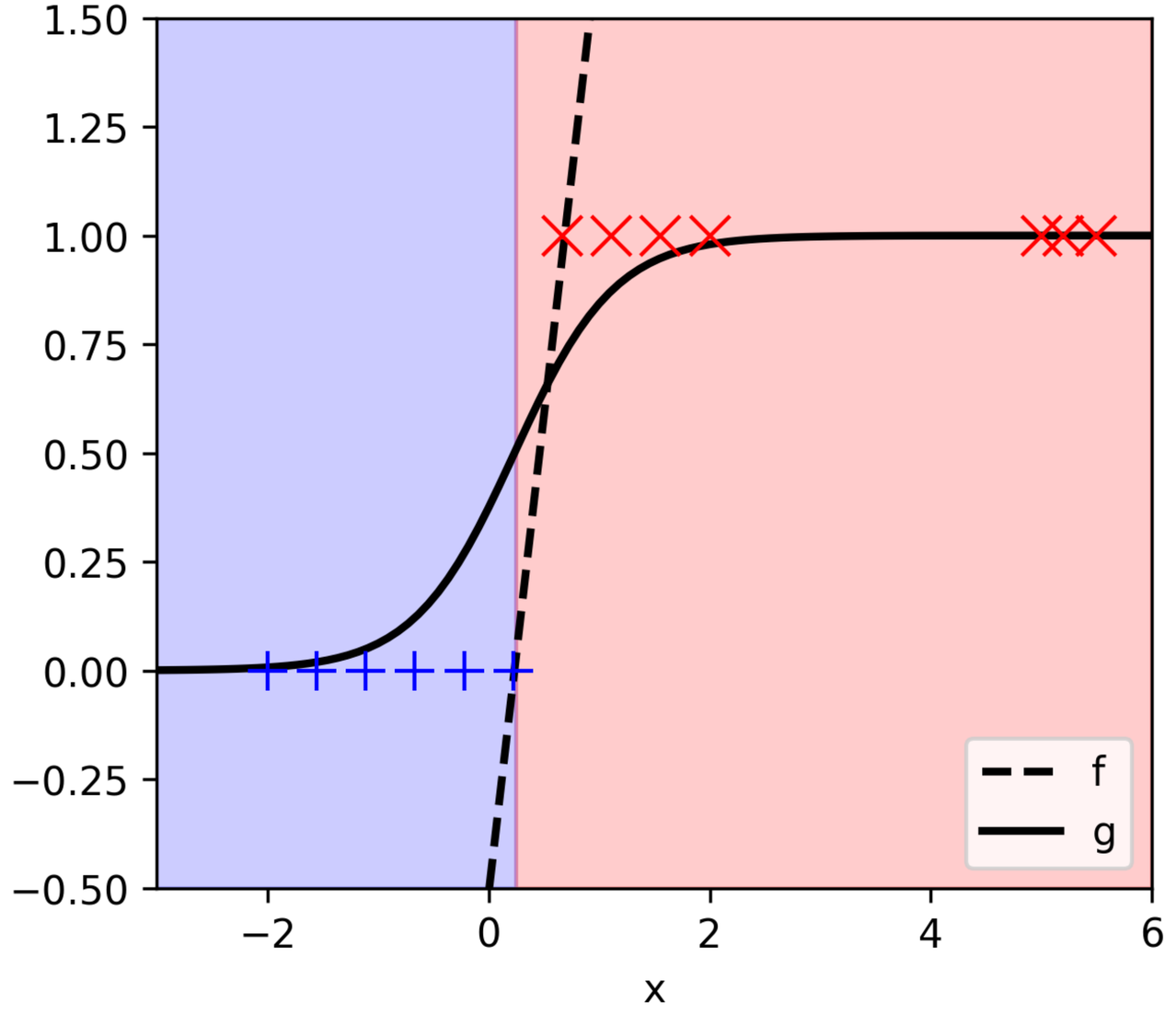

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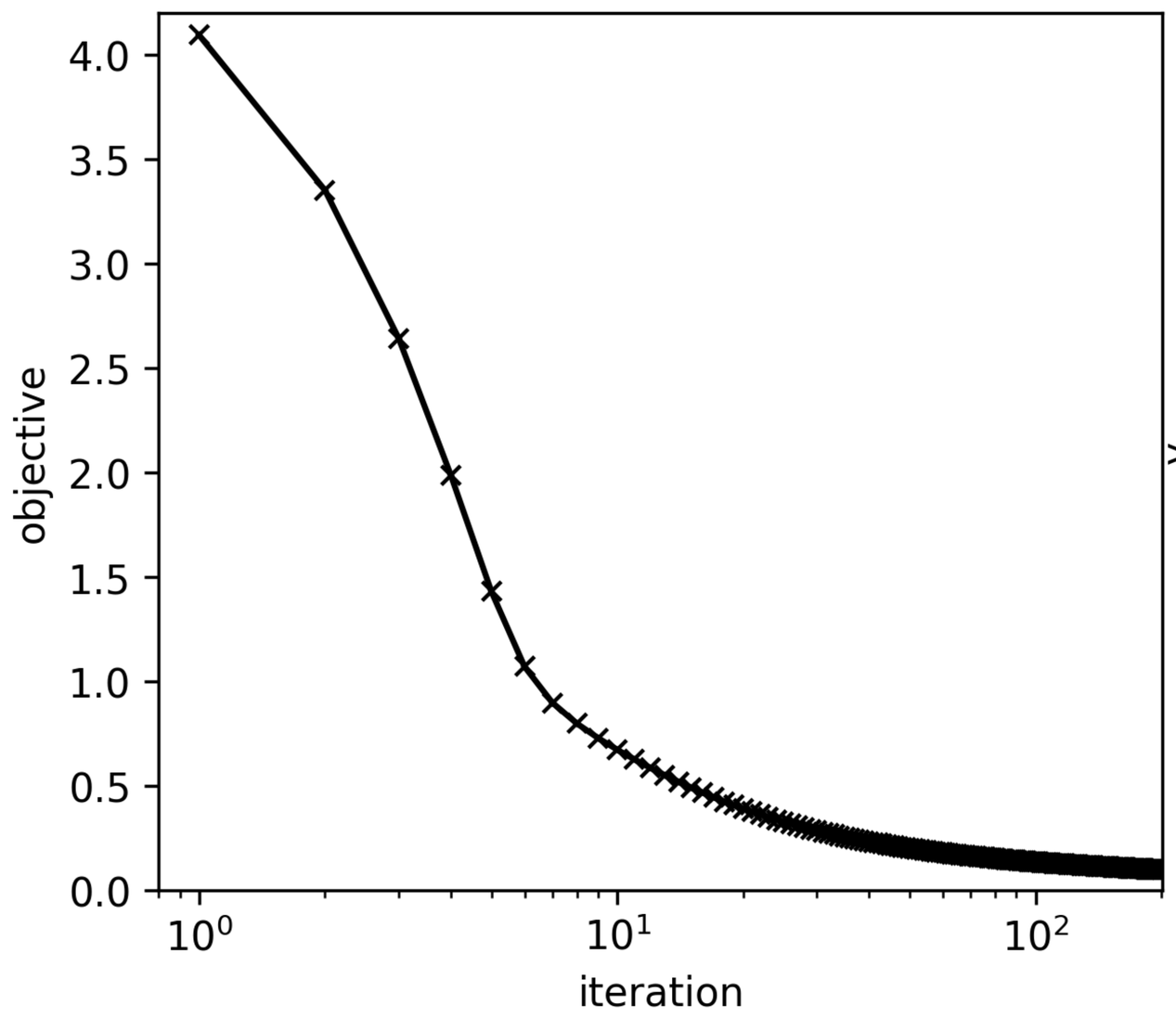

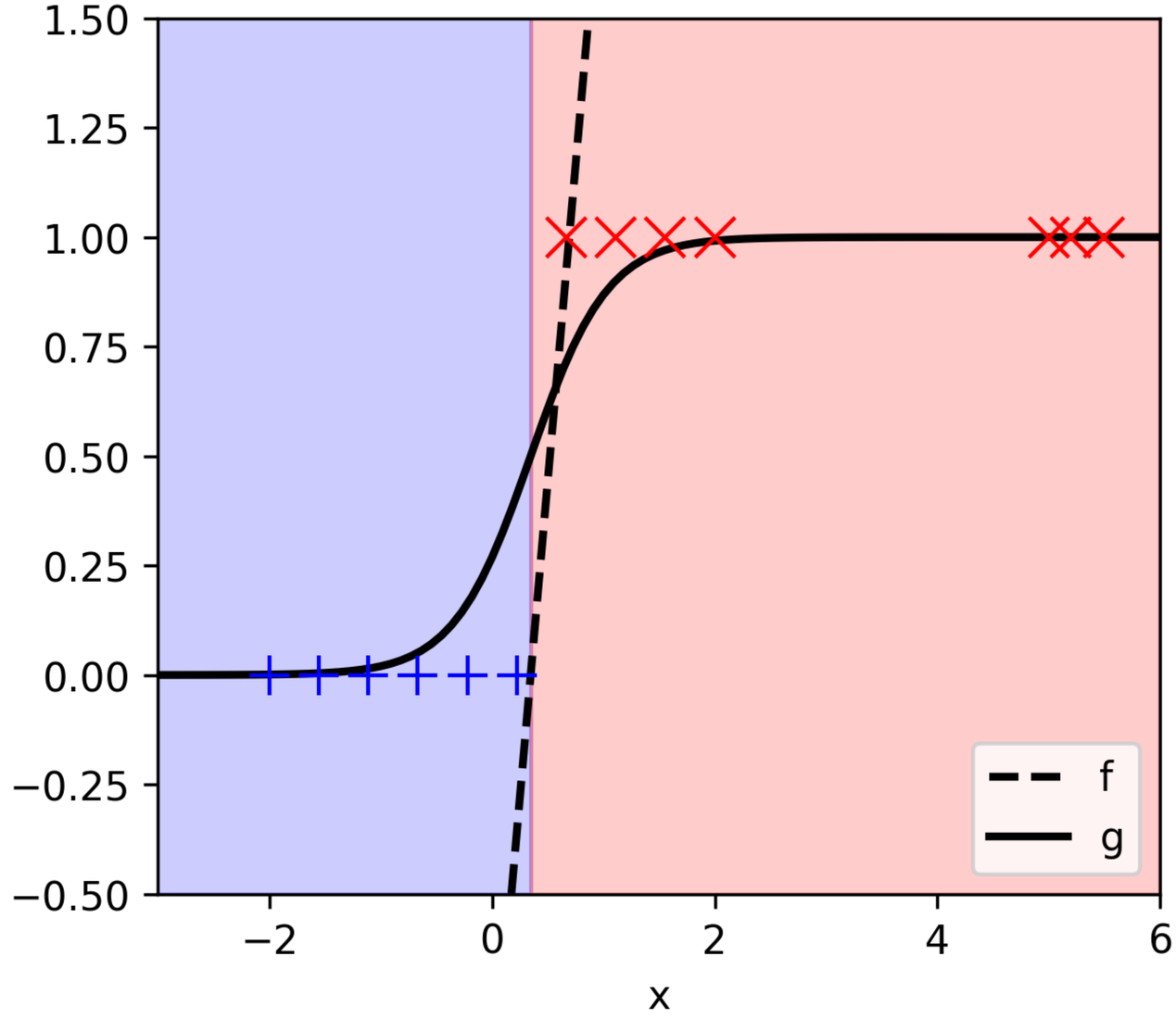

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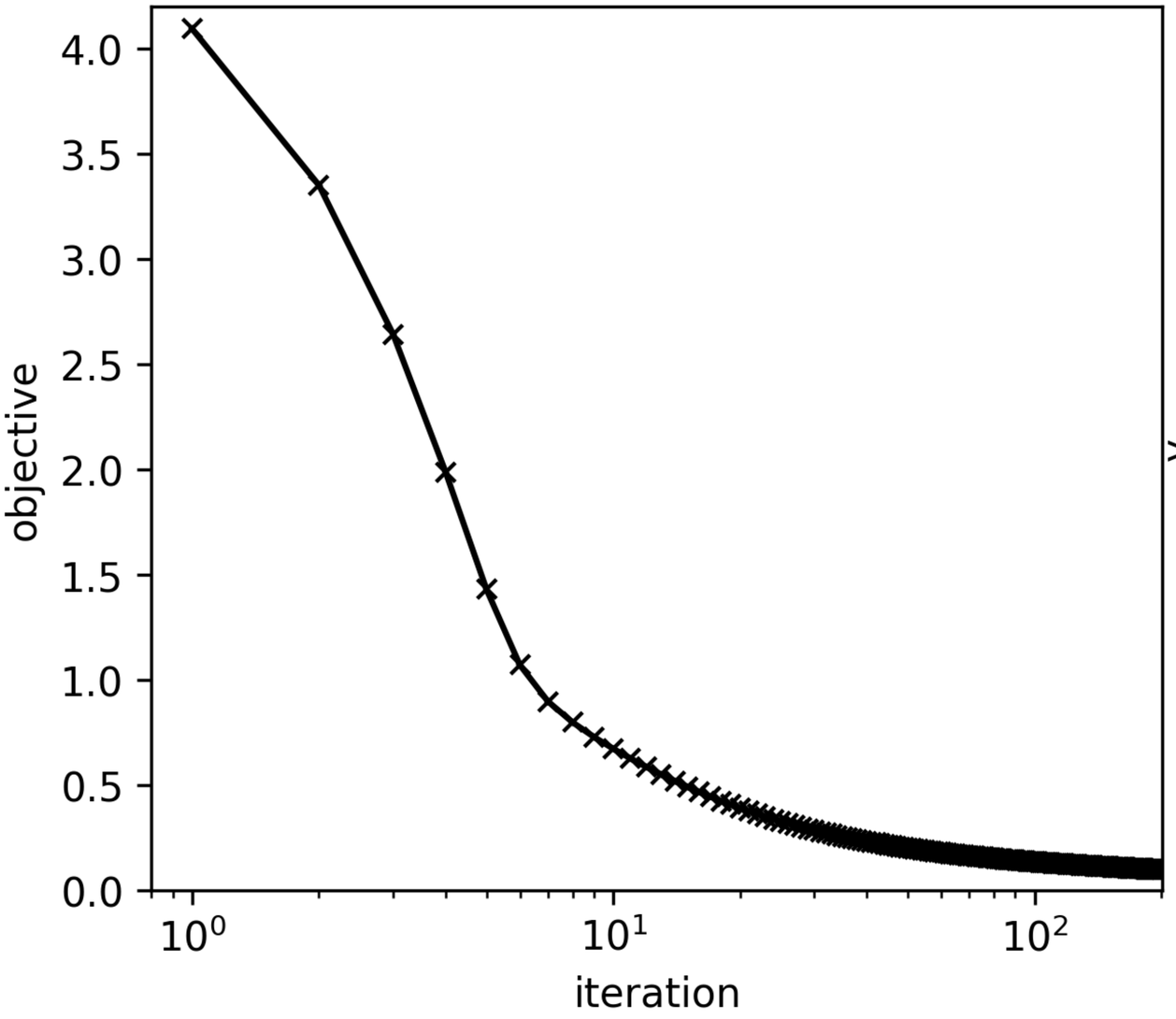

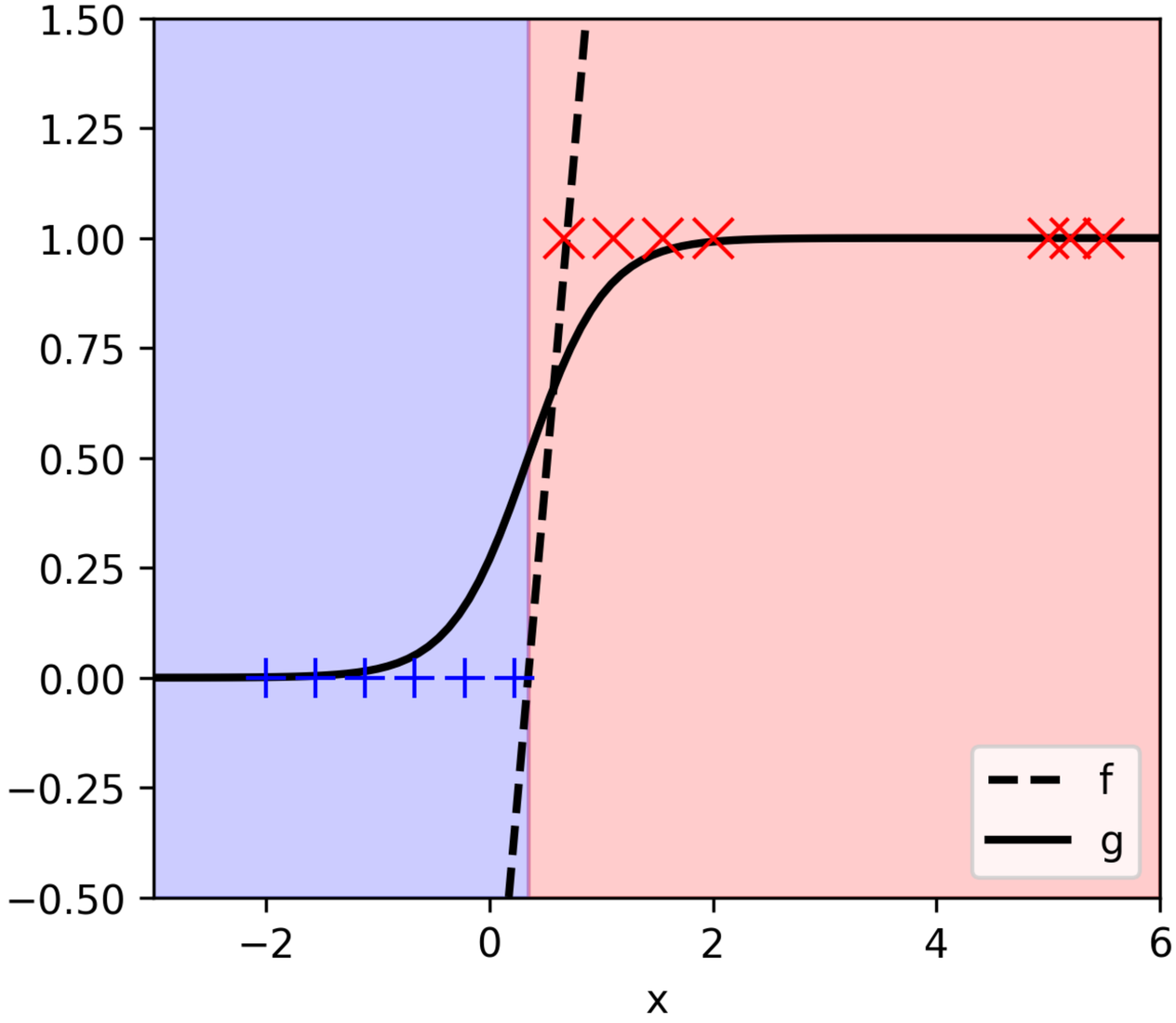

More examples: https://playground.tensorflow.org/

Binary logistic classification - benefits

Binary logistic classification - benefits

(i) Simple to implement, fast, widely used in industry

(ii) Can easily support sparse features

(iii) Easy to interpret as *log-odds* is a linear function of parameters

(iv) Easy to extend to multi-class and other kinds of outputs

(v) Easy to include new features (similar to regression) or kernelise (SML COMP4670)

Notes: often called logistic *regression*, but it is a classification task! And the underlying mapping f is still linear in the parameters.

Binary logistic classification vs linear regression

	Linear regression	Logistic regression
Underlying mapping: $f_\theta(\mathbf{x}) = \sum_{d=1}^{D} \theta_d x_d = \theta^\intercal \mathbf{x}, \theta \in \mathbb{R}^D$		**Same**
Likelihood:	$p(\mathcal{D} \mid \theta) = \prod_n \mathcal{N}(y_n; f_\theta(x_n), \sigma^2)$	$p(\mathcal{D} \mid \theta) = \prod_n \text{Bernoulli}(y_n; g_\theta(x_n))$ $g_\theta(x) = \sigma(f_\theta(x))$, σ is logistic sigmoid
Closed form: $\theta = (X^\intercal X + N\lambda \mathbf{I})^{-1} X^\intercal \mathbf{y}$ or $\theta = (X^\intercal X)^{-1} X^\intercal \mathbf{y}$		✗ **Have to use numerical optimisation**

Overview

1. Recap: Linear regression
2. From least squares to binary logistic classification
3. **From binary to multi-class classification**
4. Evaluation
5. Linearly separable data - perceptron algorithm

From binary to multi-class: set up

We construct a **classifier** that learns the class probabilities: $p(y = c \mid x)$

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From binary to multi-class: set up

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By laws of probabilities: $p(y = 1 \,|\, x) + p(y = 2 \,|\, x) + \ldots + p(y = C \,|\, x) = 1$

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Training data $\mathscr{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}, \mathbf{x}_n \in \mathbb{R}^D,\ y_n \in \{1,\ldots, C\},\ C$ classes

By laws of probabilities: $p(y = 1 \,|\, x) + p(y = 2 \,|\, x) + \ldots + p(y = C \,|\, x) = 1$

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From binary to multi-class: sigmoid to softmax

Have: $f_\theta(\mathbf{x}) = \sum_{d=1}^{D} \theta_d x_d = \theta^\intercal \mathbf{x}, \theta \in \mathbb{R}^D$. **Want:** $0 \leq g_\theta(x) \leq 1, \forall x$

Idea: 'squash' $f_\theta(x)$ through a *logistic sigmoid* function $g_\theta(x) = \sigma(f_\theta(x))$, where

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From binary to multi-class: cross-entropy

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minimise negative log-likelihood

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Often called the **binary cross-entropy loss**

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If *one-hot coding or 1-of-C coding* is used, $\mathbf{t}_n = (t_{n1}, t_{n2}, \ldots, t_{nC})$

where $t_{nc} = 1$ if $y_n = c$ and 0 otherwise:

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One-vs-one approach

- A binary classifier is built for every pairwise combination of classes. A total of $\frac{C(C-1)}{2}$ classifiers for C classes.
- Each classifier receives the samples of a pair of classes from the original training set, and learns to distinguish these two classes.
- At prediction time, a voting scheme is applied: all $\frac{C(C-1)}{2}$ classifiers are applied and the class that has the highest number of **1** predictions is chosen by the combined classifier.

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One-vs-all (one-vs-rest) approach

- Classifier is built for each class and the remaining classes are grouped into one large "negative" class. A total of C binary classifiers.
- For a new case x^*, predicting the label c for which the corresponding classifier has the highest confidence score (e.g., the probability in logistic regression)

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Binary classification - confusion matrix

True label

Predicted label	$y = -1$	$y = 1$	Total
$\hat{y} = -1$			
$\hat{y} = 1$			
Total			

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Predicted label	$y = -1$	$y = 1$	Total
$\hat{y} = -1$	True negative (TN)		
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Binary classification - confusion matrix

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Predicted label	$y = -1$	$y = 1$	Total
$\hat{y} = -1$	True negative (TN)		
$\hat{y} = 1$		True positive (TP)	
Total			

Binary classification - confusion matrix

		True label		
		$y = -1$	$y = 1$	Total
Predicted label	$\hat{y} = -1$	True negative (TN)		
	$\hat{y} = 1$	False positive (FP)	True positive (TP)	
	Total			

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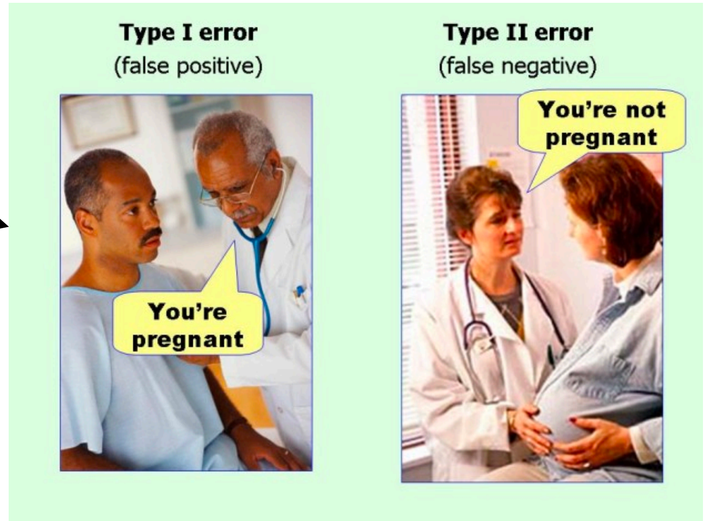

Binary classification - popular metrics

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$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{N} \qquad \text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} \qquad \text{True positive rate (TPR)} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{Error} = \frac{\text{FP} + \text{FN}}{N} \qquad \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \qquad \text{False positive rate (FPR)} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

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Questions: compute these metrics for

1. A perfect classifier
2. All classified as positive
3. All classified as negative
4. Random guessing

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Binary classification - too many metrics?

Ratio	Name
FP/N	False positive rate, Fall-out, Probability of false alarm
TN/N	True negative rate, Specificity, Selectivity
TP/P	True positive rate, Sensitivity, Power, *Recall*, Probability of detection
FN/P	False negative rate, Miss rate
TP/P*	Positive predictive value, *Precision*
FP/P*	False discovery rate
TN/N*	Negative predictive value
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P/*n*	Prevalence
(FN + FP)/*n*	*Misclassification rate*
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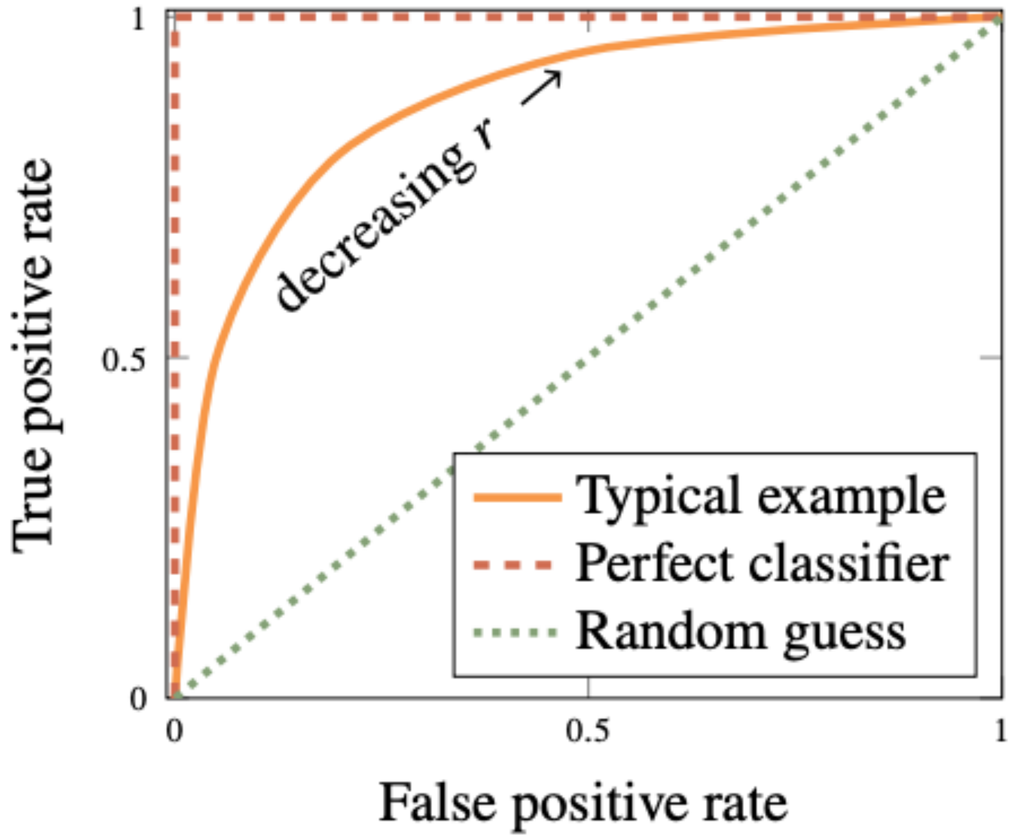
In this table: N is Nn, P is Np, n is N

Binary classification - Receiver Operating Characteristic



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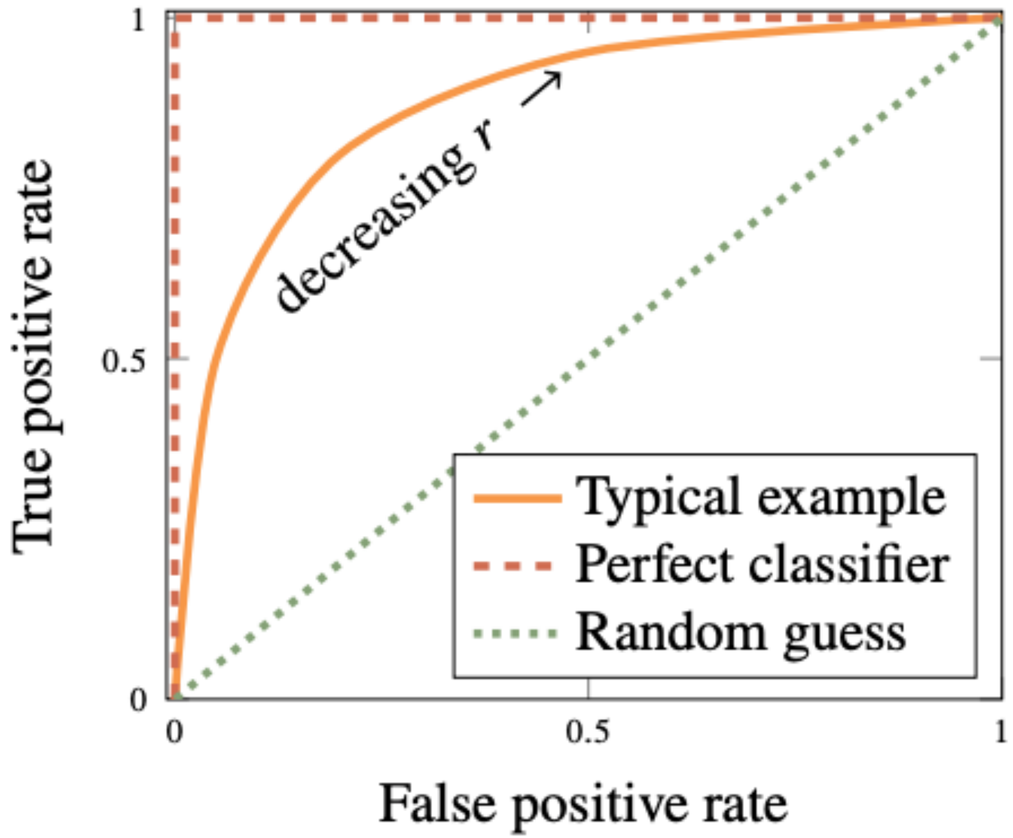

Consider a binary classification example, at test time:

$$p(y^* = 1 \,|\, x^*) = g(x^*) \text{ and } p(y^* = 0 \,|\, x^*) = 1 - g(x^*)$$

We choose a **decision threshold** r and decide:

$$y^* = \begin{cases} 1 & \text{if } g(x^*) > r \\ 0 & \text{otherwise} \end{cases}$$

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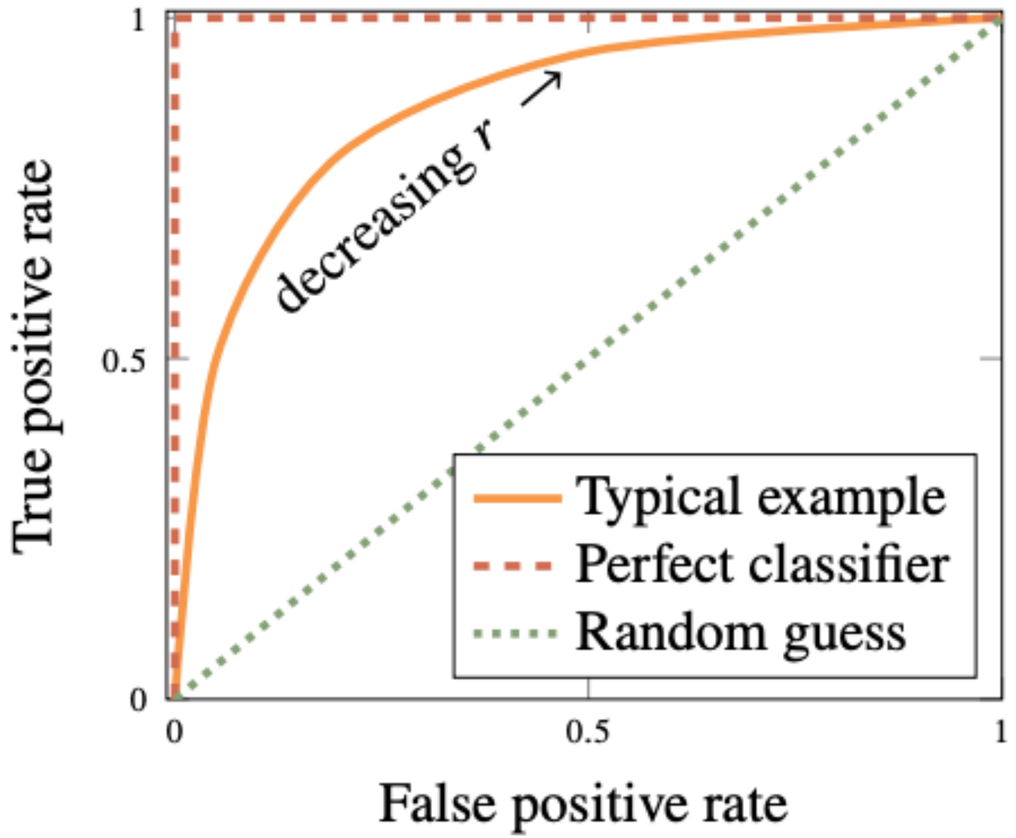

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Join the points for all thresholds to form the ROC curve.

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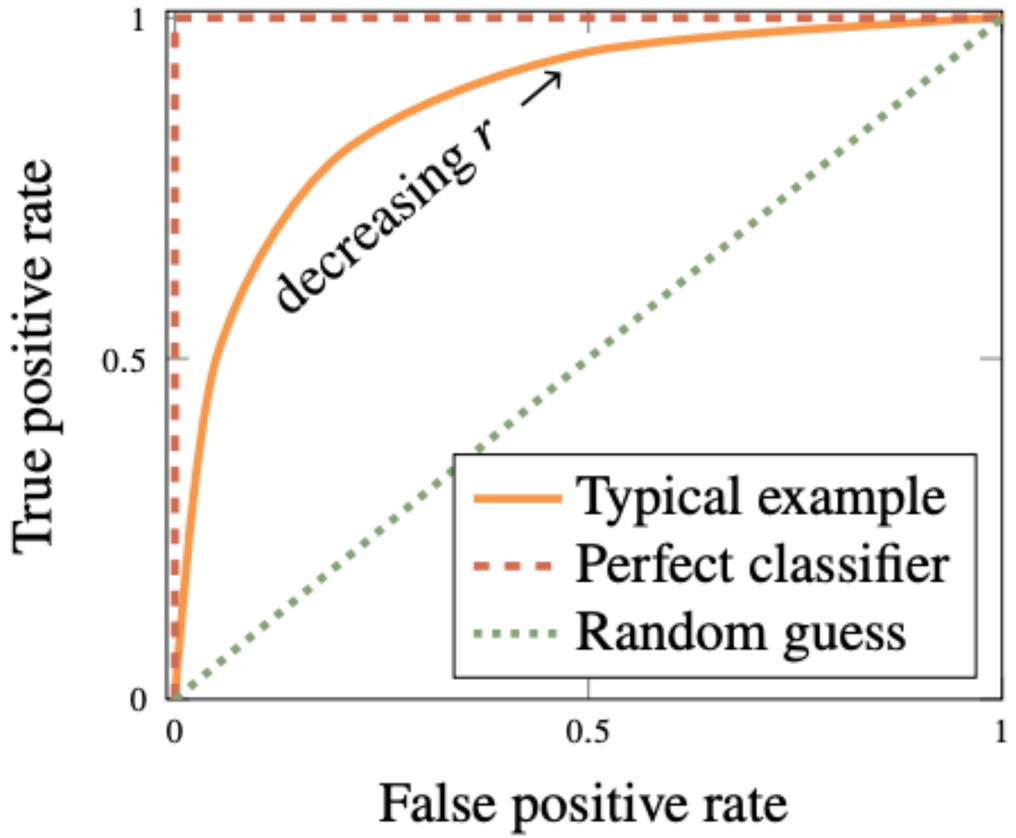

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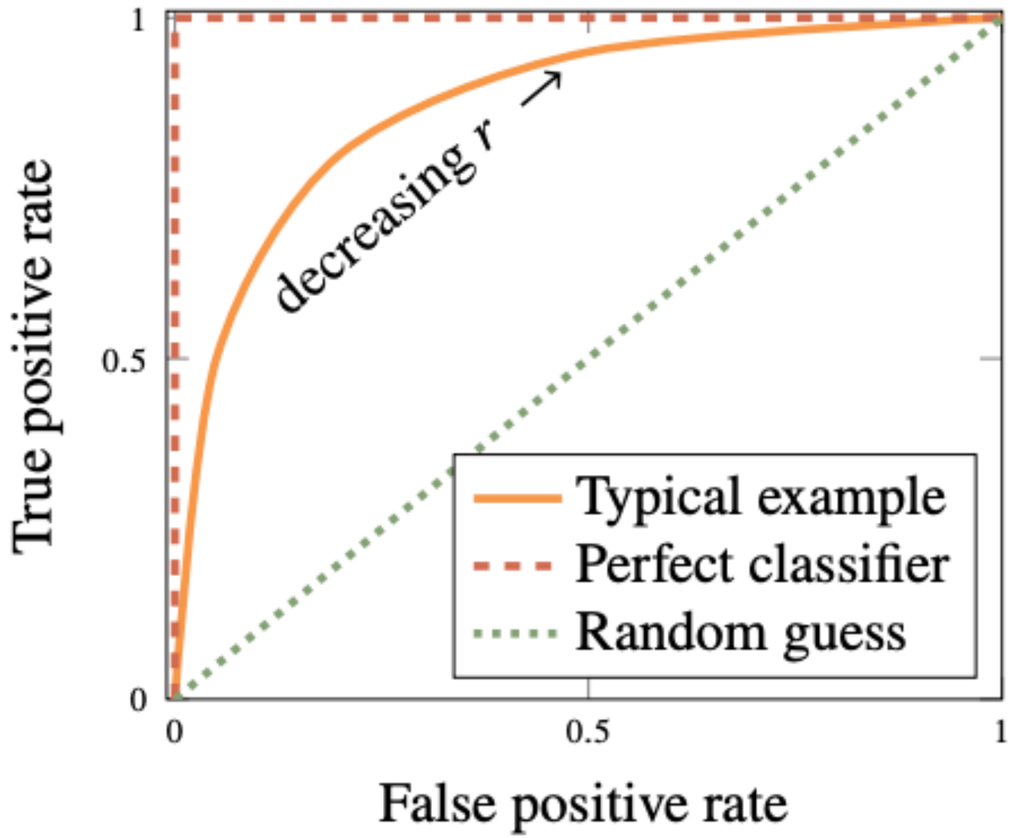

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For imbalanced data (with many negatives), we can use **precision-recall curve** instead.

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5. **Linearly separable data - perceptron algorithm**

Rosenblatt

Frank Rosenblatt
1928–1969

Rosenblatt's perceptron played an important role in the history of machine learning. Initially, Rosenblatt simulated the perceptron on an IBM 704 computer at Cornell in 1957, but by the early 1960s he had built special-purpose hardware that provided a direct, parallel implementation of perceptron learning. Many of his ideas were encapsulated in "Principles of Neurodynamics: Perceptrons and the Theory of Brain Mechanisms" published in 1962. Rosenblatt's work was criticized by Marvin Minksy, whose objections were published in the book "Perceptrons", co-authored with Seymour Papert. This book was widely misinterpreted at the time as showing that neural networks were fatally flawed and could only learn solutions for linearly separable problems. In fact, it only proved such limitations in the case of single-layer networks such as the perceptron and merely conjectured (incorrectly) that they applied to more general network models. Unfortunately, however, this book contributed to the substantial decline in research funding for neural computing, a situation that was not reversed until the mid-1980s. Today, there are many hundreds, if not thousands, of applications of neural networks in widespread use, with examples in areas such as handwriting recognition and information retrieval being used routinely by millions of people.

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Perceptron model: $y_n = \begin{cases} 1, & \text{if } \theta^\intercal x_n \geq 0 \\ -1 & \text{if } \theta^\intercal x_n < 0 \end{cases}$

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$g_\theta(x) = \sigma(f_\theta(x))$, σ is logistic sigmoid

Perceptron model: $y_n = \begin{cases} 1, & \text{if } \theta^\intercal x_n \geq 0 \\ -1 & \text{if } \theta^\intercal x_n < 0 \end{cases}$

Perceptron criterion: Want $y_n \theta^\intercal x_n > 0$ for all n, $L(\theta) = -\sum_{n \in \mathscr{M}} y_n \theta^T x_n$

$\mathscr{M}$: all mis-classified examples

Perceptron - learning algorithm

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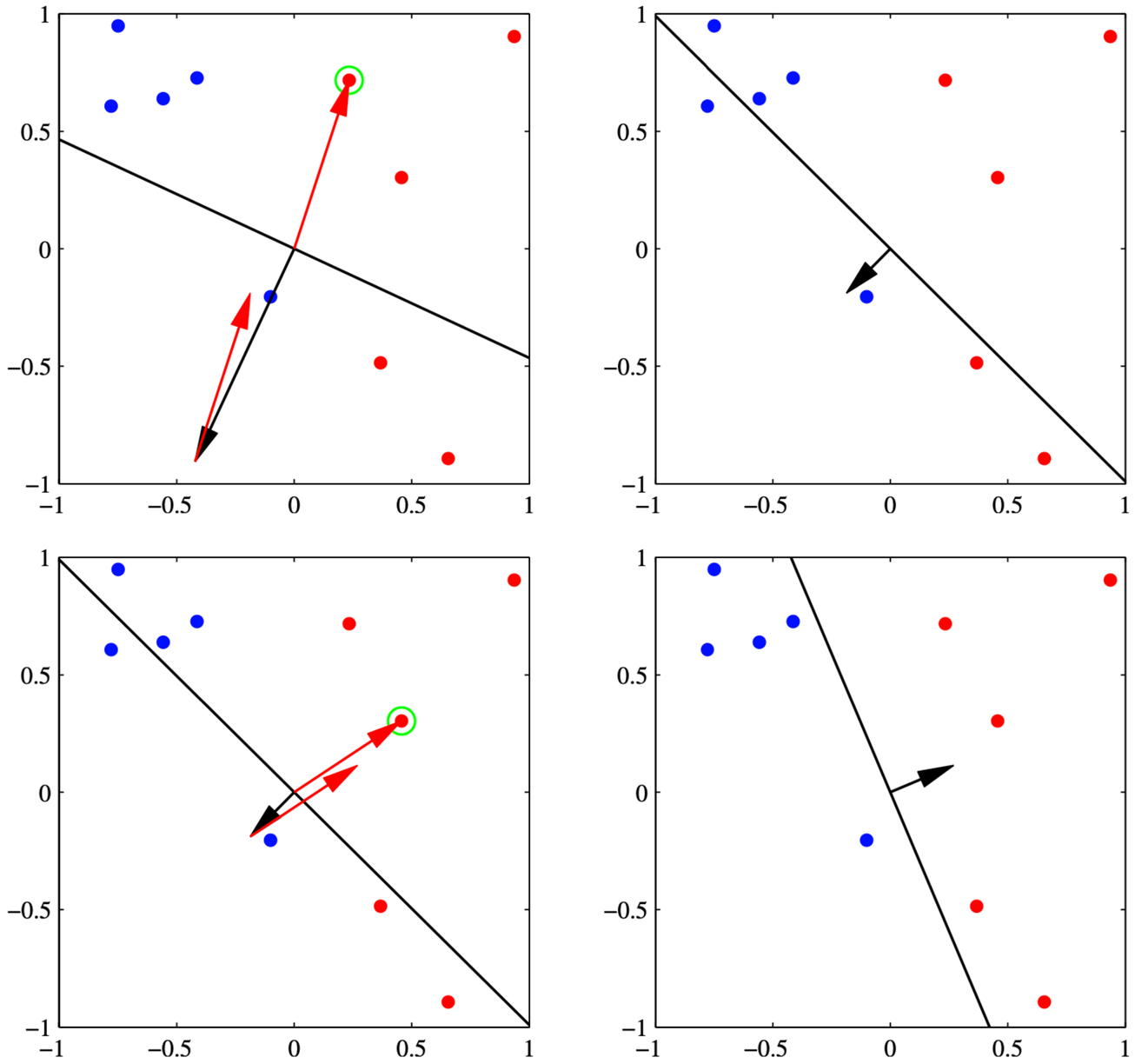
$\mathcal{M}$: all mis-classified examples

SGD update: *for each misclassified example,* $\theta^{t+1} = \theta^t + x_n y_n$. Derive this!

Perceptron algorithm - an example



PRML Bishop

Perceptron - potential issues

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The perceptron *does not* provide probabilistic outputs, nor does it generalise readily to $K > 2$ classes

Whew :) That's it! Well, not quite :(

- *Assignment 4* is now available on Wattle (due next week - W12 Monday)
- *Exam* timetable is available.
  - Check time + location
  - Past exam papers released on Wattle
- Guest lecture: W12 Monday October 23
  - Dr Zheng Yuan, King's College London
  - *Examinable*!
  - Please do show up!
- Review lecture next Wed