Logistic classification

Week 3a - Statistical ML / Thang Bui / ANU / 2025 S1

Housekeeping

+ Assignment 1 was released on Friday, due in <4 weeks [mid-night Fri 28/3].

+ 20% of total. 5% penalty for 5 mins - 24 hrs late, 100% penalty after.

+ We use Ed for discussion. Sign-up link is in Wattle/Vital Information.

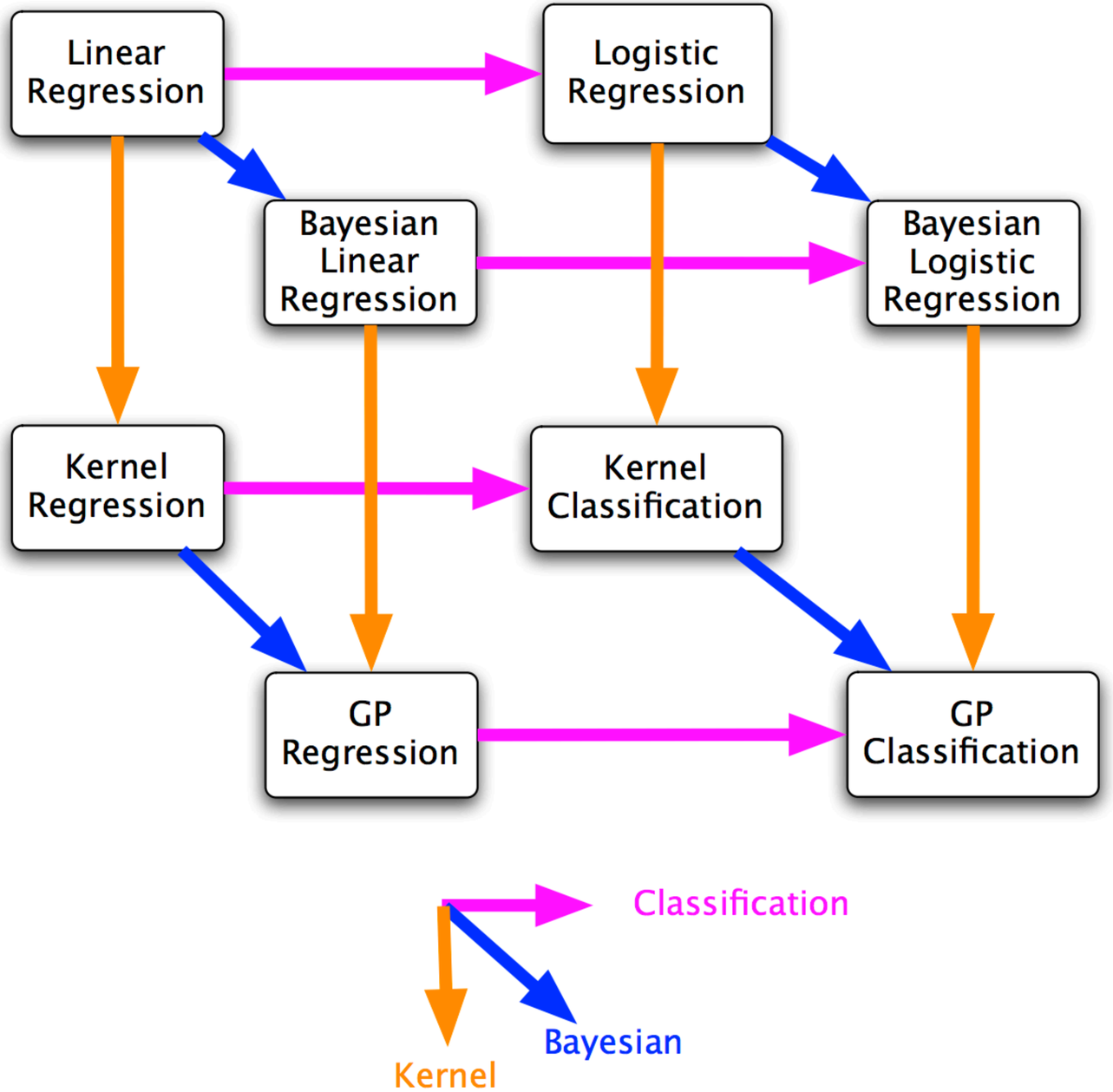
+ Class reps: Liam Engler, Arjun Raj, Harold Gao, and Wenyu Dai.

+ If you have questions, we are here to help [through Ed + consultation/office hours].

+ Feel free to ask questions during the lectures

+ Any burning administrative issues after 2 weeks? What worked/didn’t work?

Big picture of the first six weeks of SML



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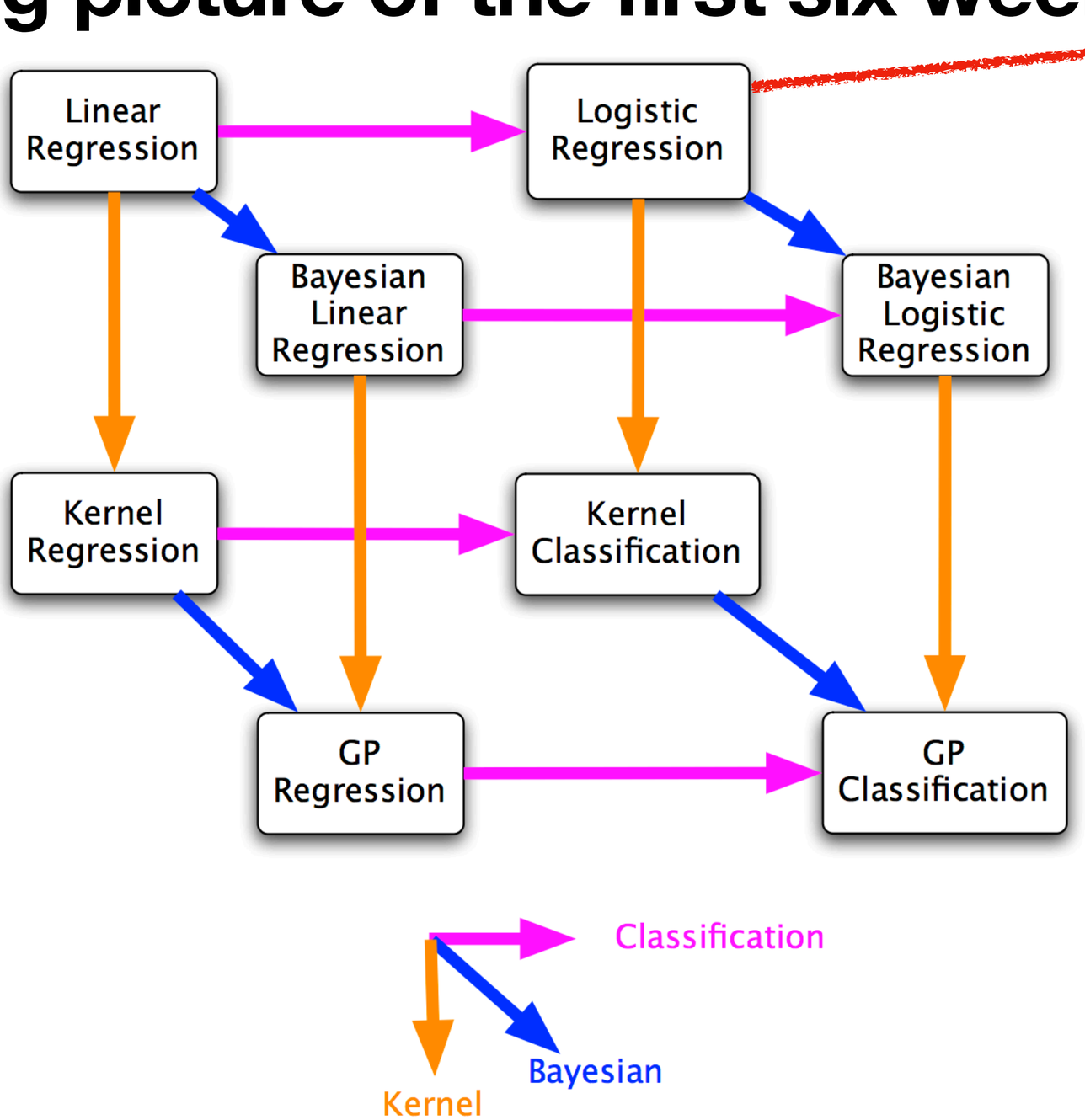

Overview

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Three approaches to classification:

Learning a discriminant function, directly mapping $\mathbf{x}$ to class label y

Building a discriminative model, learning $p_\theta(\mathbf{y} \mid \mathbf{x})$

Building a generative model, learning $p_\theta(\mathbf{x} \mid \mathbf{y})$ and $p_\phi(\mathbf{y})$ then find $p_{\theta,\phi}(\mathbf{y} \mid \mathbf{x})$ using Bayes' rule.

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Least squares [Bishop 4.1.3],
Perceptron for linearly separable data [Bishop 4.1.7]

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logistic classification [Bishop 4.3],
Non-linear models such as GP or neural network classification

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Gaussian/Linear discriminant analysis [Bishop 4.2.1],
Naive Bayes classifier

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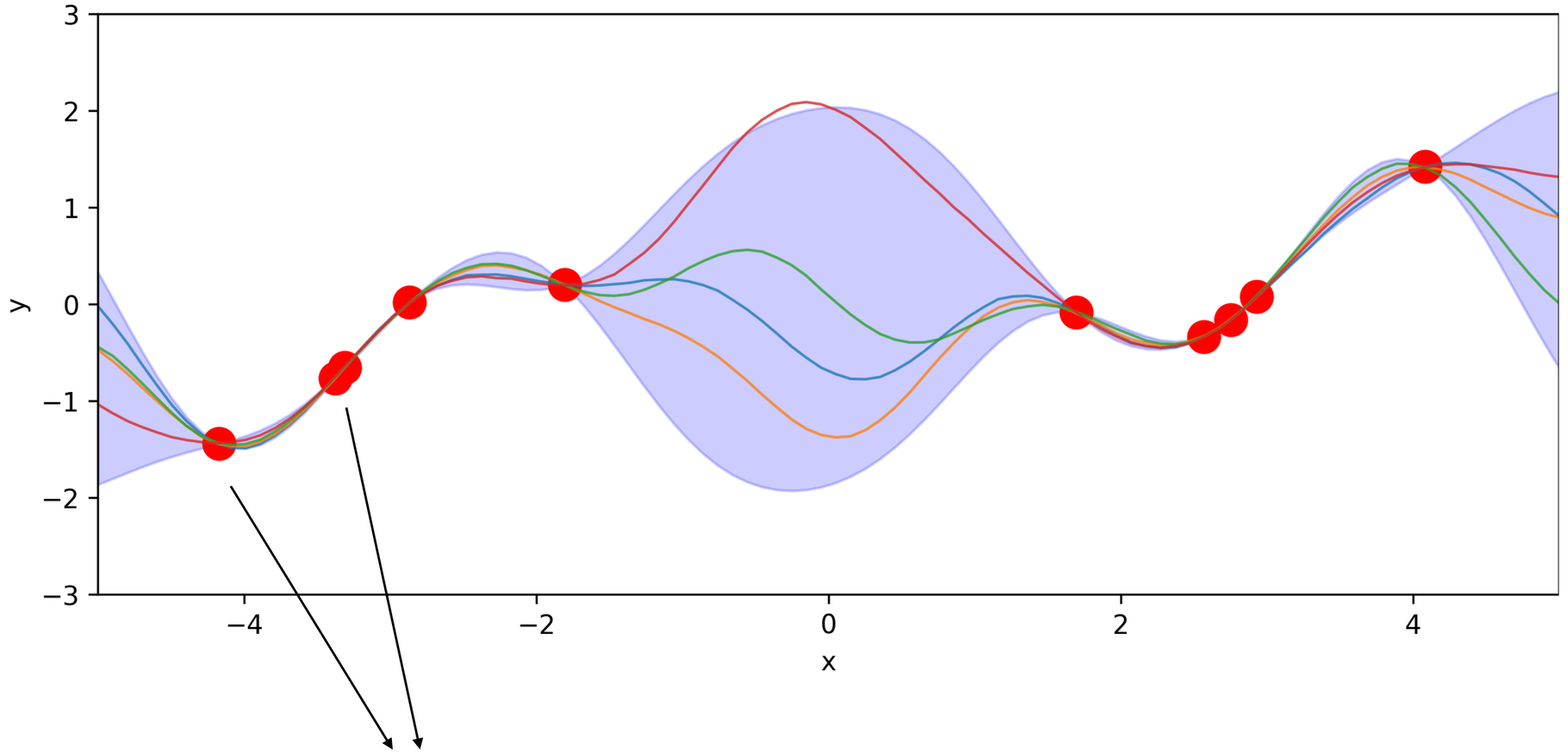
Today

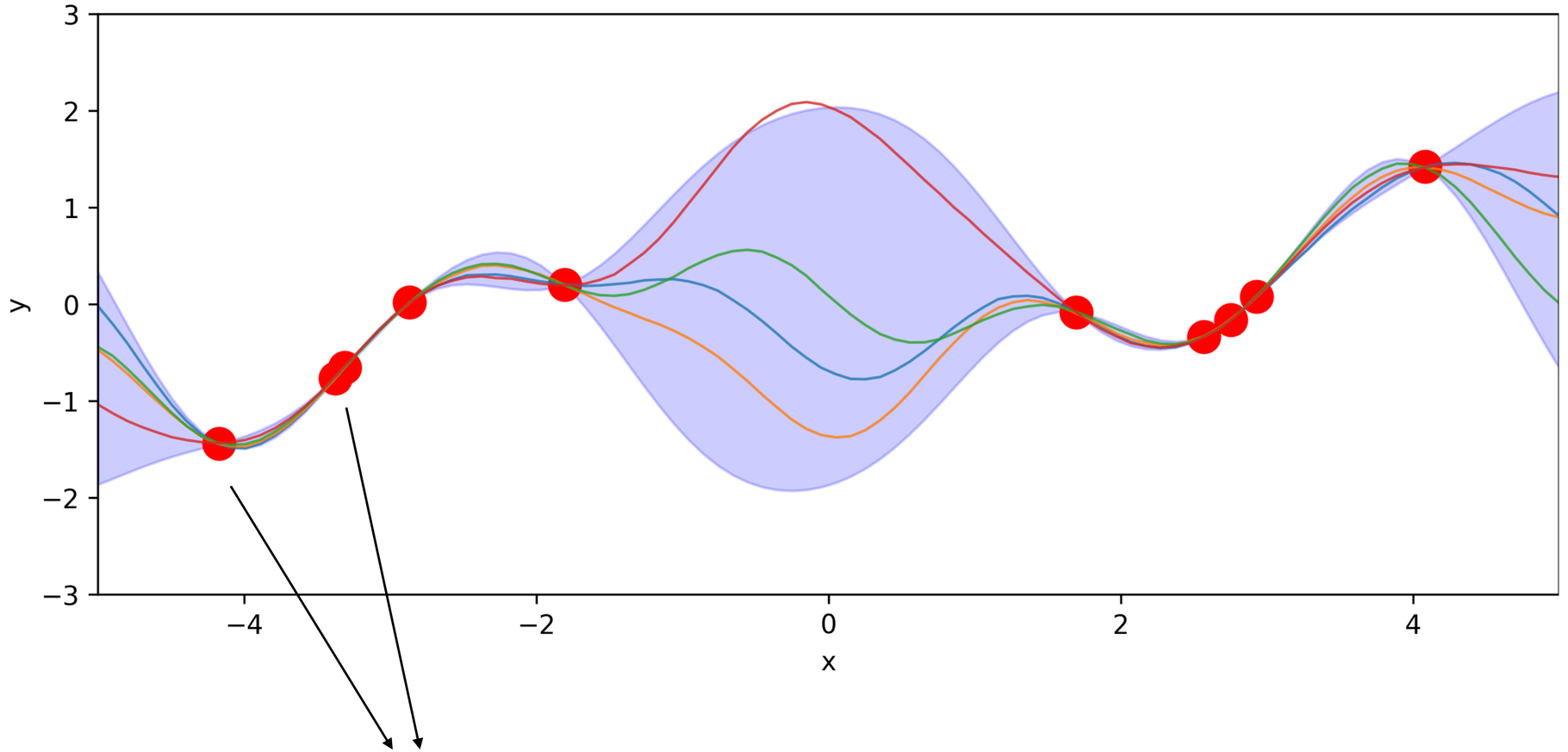
1. *Discriminative linear* models: From least squares to binary logistic classification, and from binary to multi-class classification
2. A generative classifier: Linear discriminant analysis
3. At-home: Evaluation and the Perceptron algorithm

Recap: regression and linear regression



Observed data

Recap: regression and linear regression



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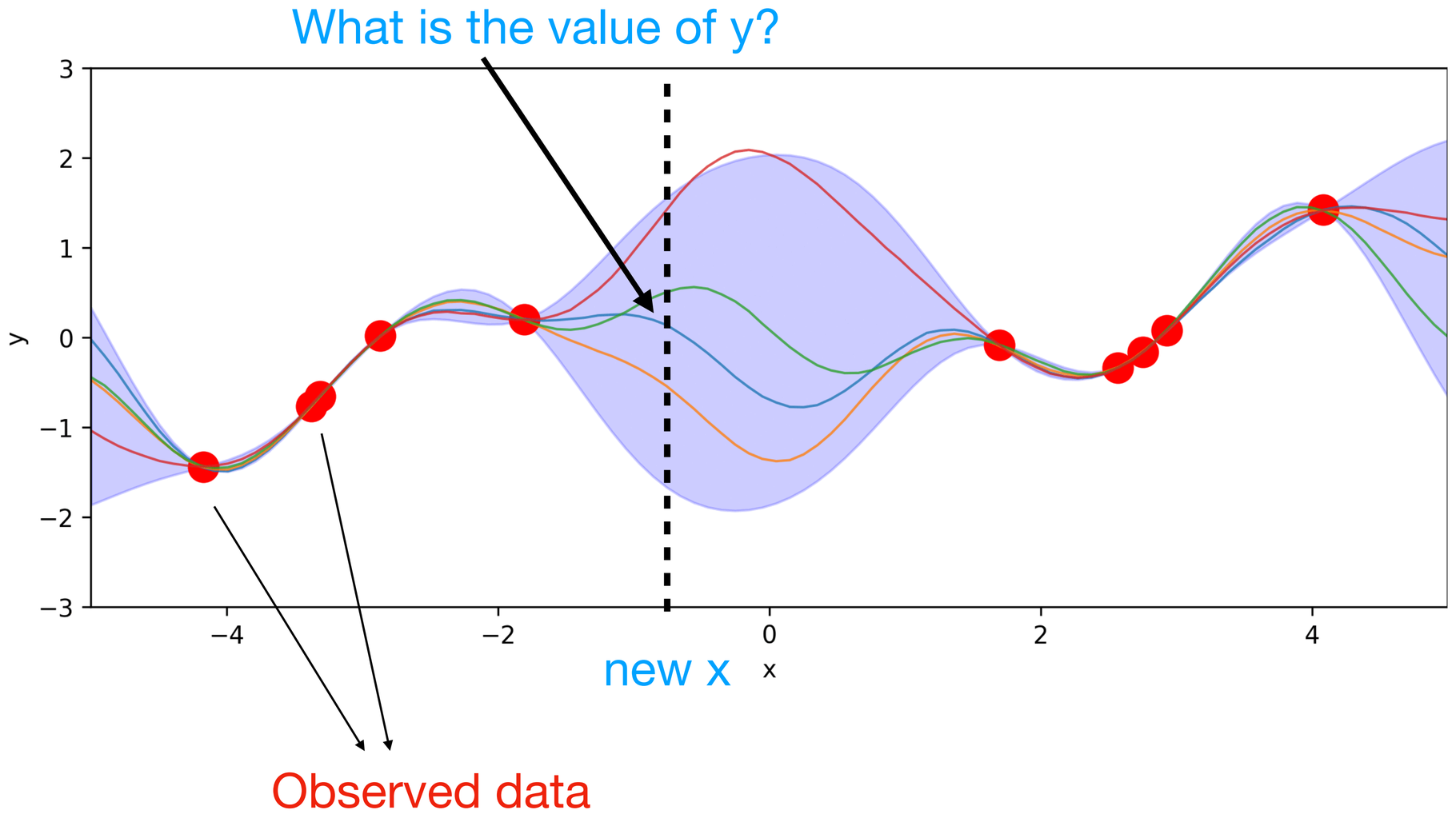

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Training data N input, output pairs $\mathcal{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}, \mathbf{x}_n \in \mathbb{R}^D, y_n \in \mathbb{R}$

Each row is a data point

Each column is a feature dimension

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One scalar per data point

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- Underlying function is **linear**, $f_\theta(\mathbf{x}) = \sum_{d=1}^{D} \theta_d x_d = \theta^\intercal \mathbf{x}, \theta \in \mathbb{R}^D$

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

Finding θ

Likelihood: $p(\mathcal{D}\,|\,\theta) = \prod_n \mathcal{N}(y_n; f(x_n), \sigma^2) = \prod_n \mathcal{N}(y_n; x_n^\intercal \theta, \sigma^2) = \mathcal{N}(\mathbf{y}; \mathbf{X}\theta, \sigma^2 \mathrm{I}_N)$

Prior: $p(\theta) = \mathcal{N}(\theta; \mu_o, \Sigma_o)$ We choose a Gaussian prior for simplicity and analytic tractability

Exact Bayesian inference: $p(\theta\,|\,\mathcal{D}) = \mathcal{N}(\theta; \mu, \Sigma)$

$$\mu = \mu_o + \Sigma_o \mathbf{X}^\intercal (\mathbf{X}\Sigma_o \mathbf{X}^\intercal + \sigma^2 \mathrm{I})^{-1}(\mathbf{y} - \mathbf{X}\mu_o)$$

$$\Sigma = \Sigma_o - \Sigma_o \mathbf{X}^\intercal (\mathbf{X}\Sigma_o \mathbf{X}^\intercal + \sigma^2 \mathrm{I})^{-1}\mathbf{X}\Sigma_o$$

MAP: $\mu_o = 0,\ \Sigma_o = \frac{\sigma^2}{\lambda}\mathrm{I},\ \mu = (\mathbf{X}^\intercal\mathbf{X} + \lambda \mathrm{I})^{-1}\mathbf{X}^\intercal\mathbf{y}.$

Maximum likelihood: $\mu_o = 0,\ \Sigma_o = \frac{\sigma^2}{\lambda}\mathrm{I},\ \lambda \to 0,\ \mu = (\mathbf{X}^\intercal\mathbf{X})^{-1}\mathbf{X}^\intercal\mathbf{y}.$

Linear regression - an example

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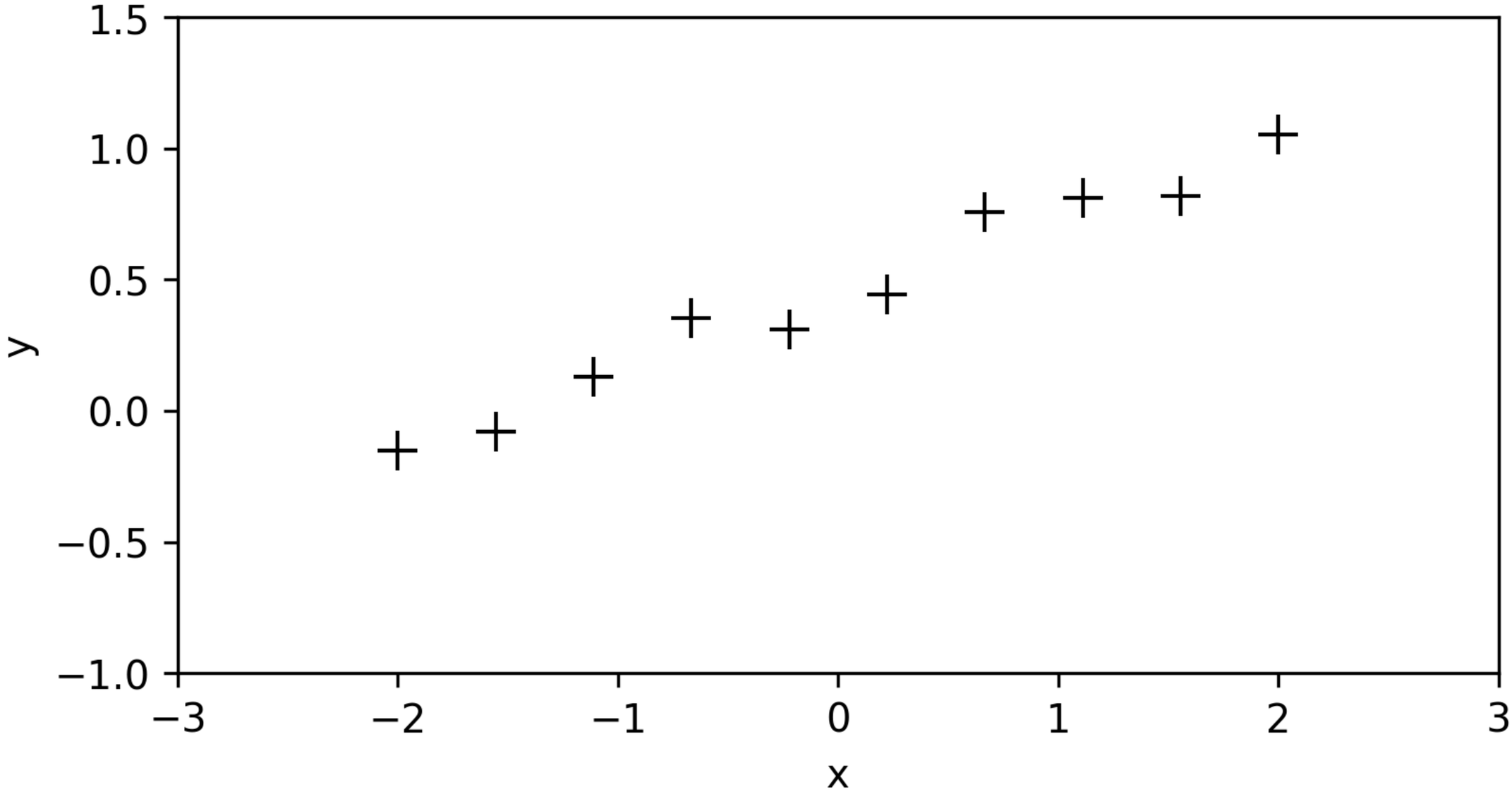

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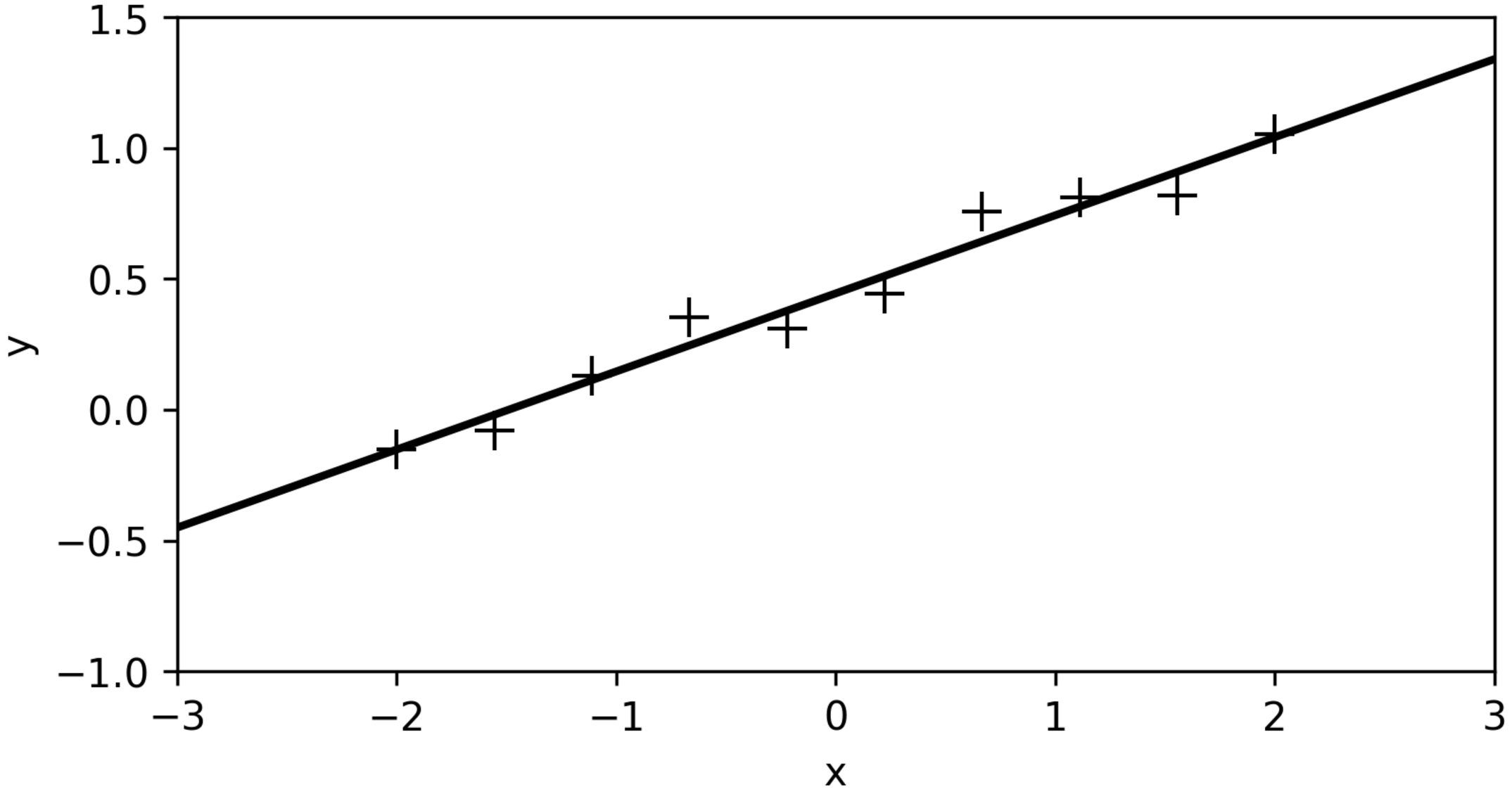

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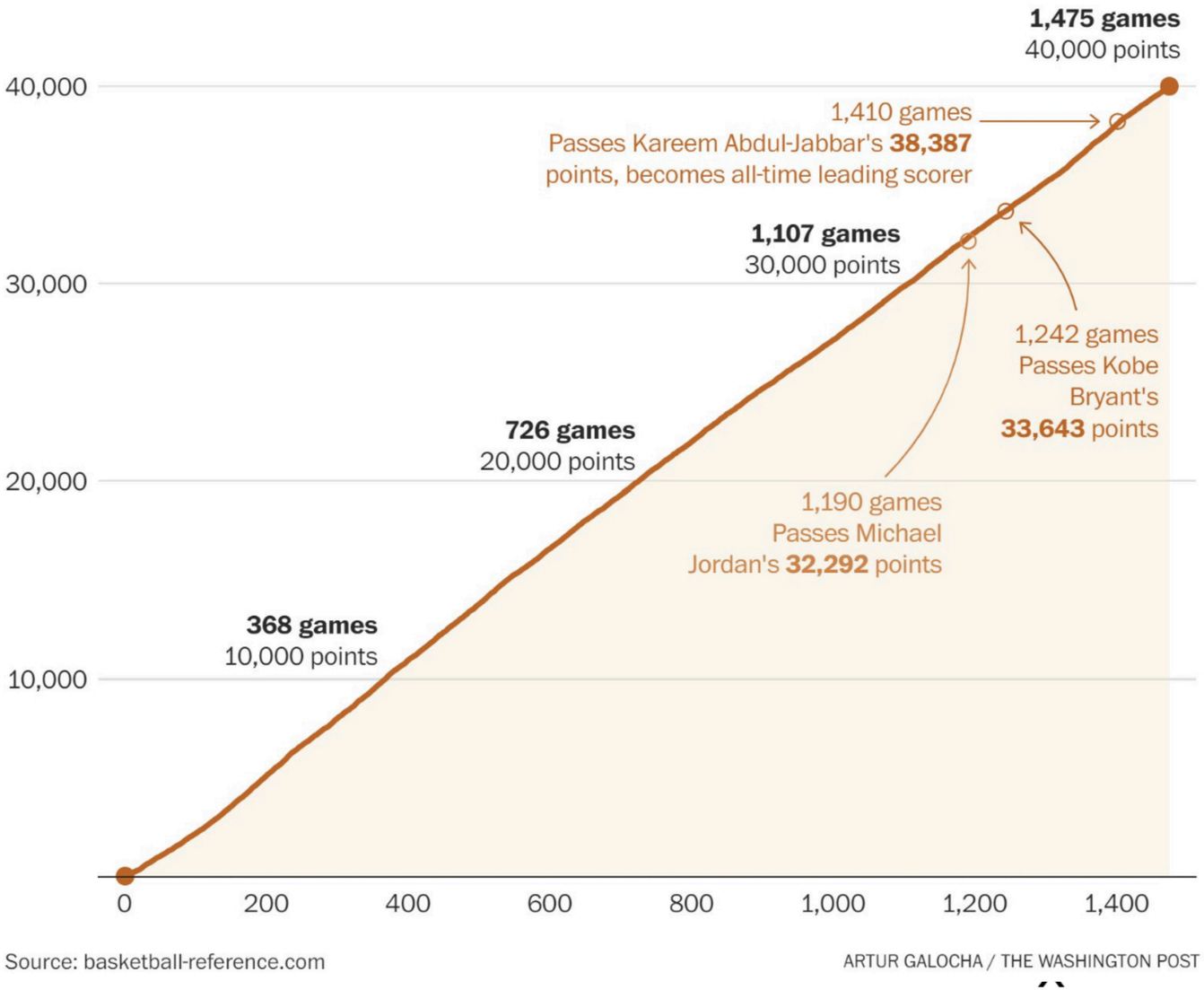

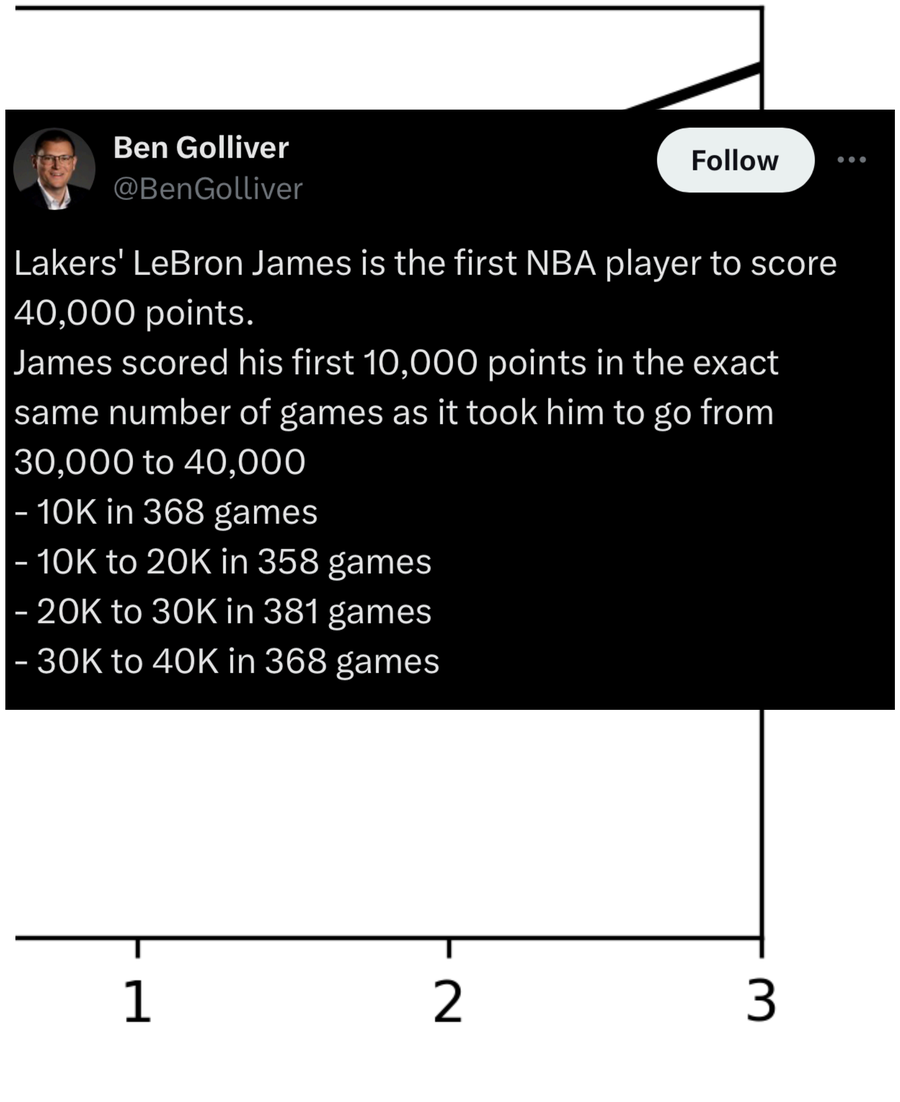

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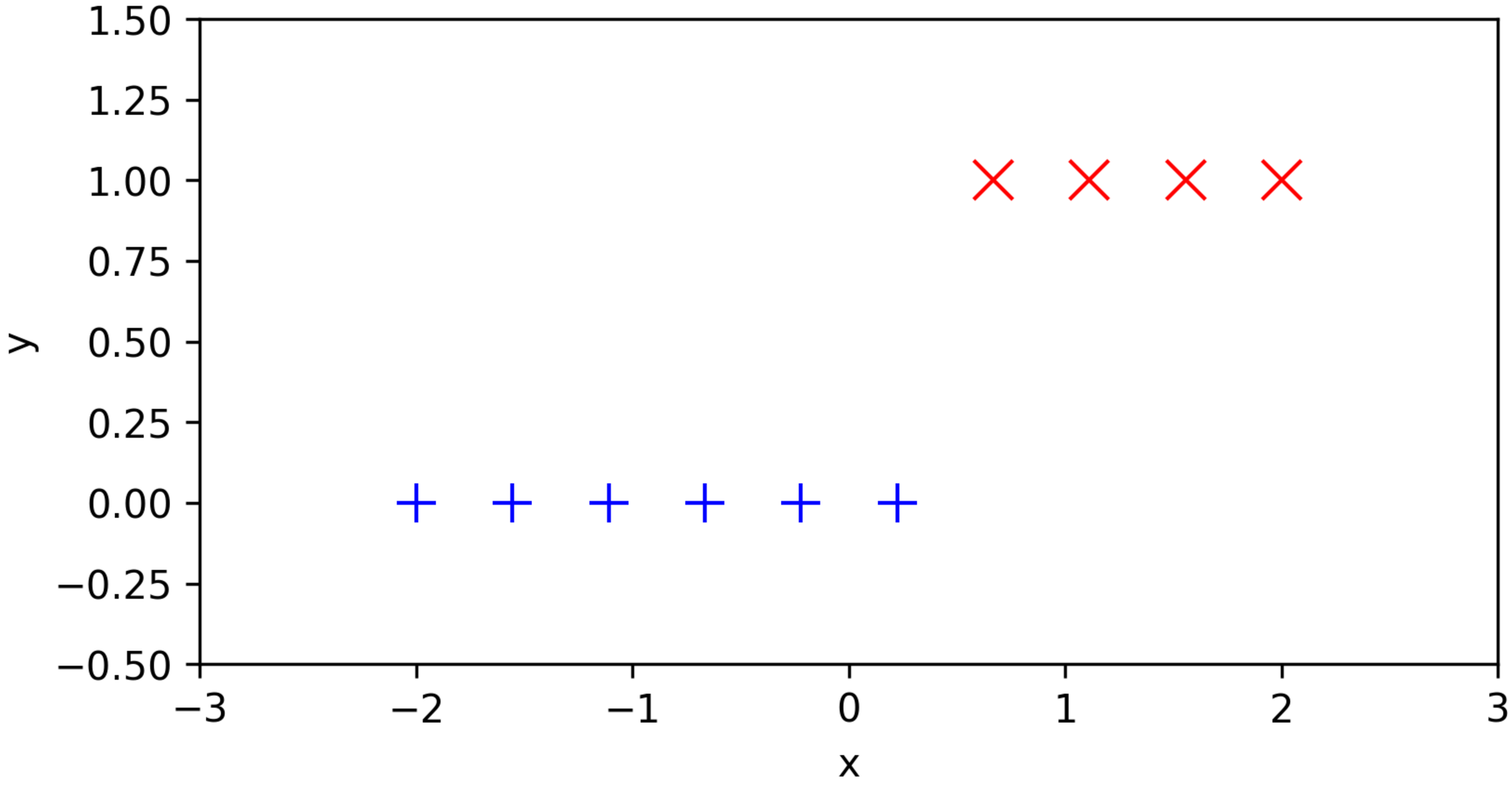

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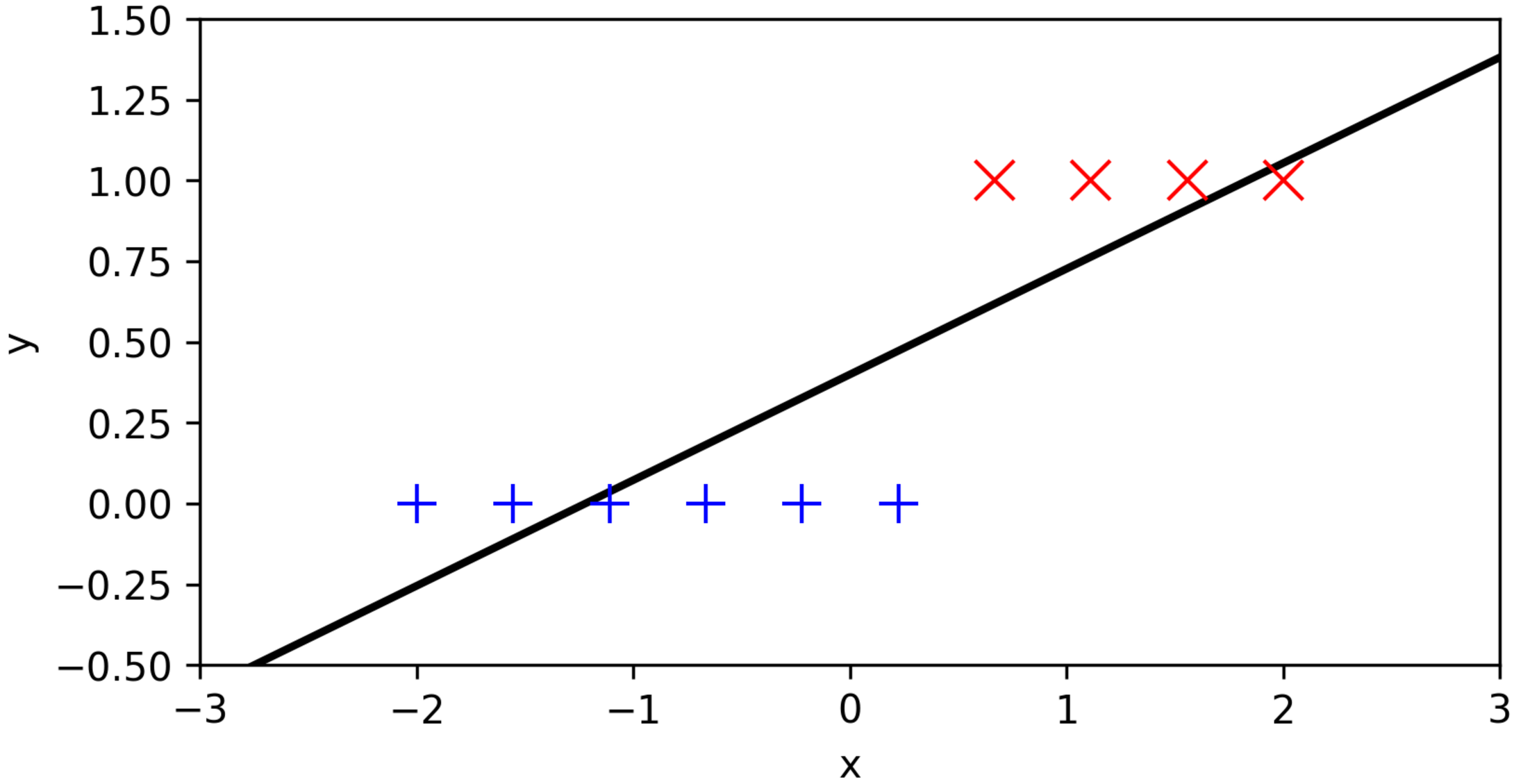

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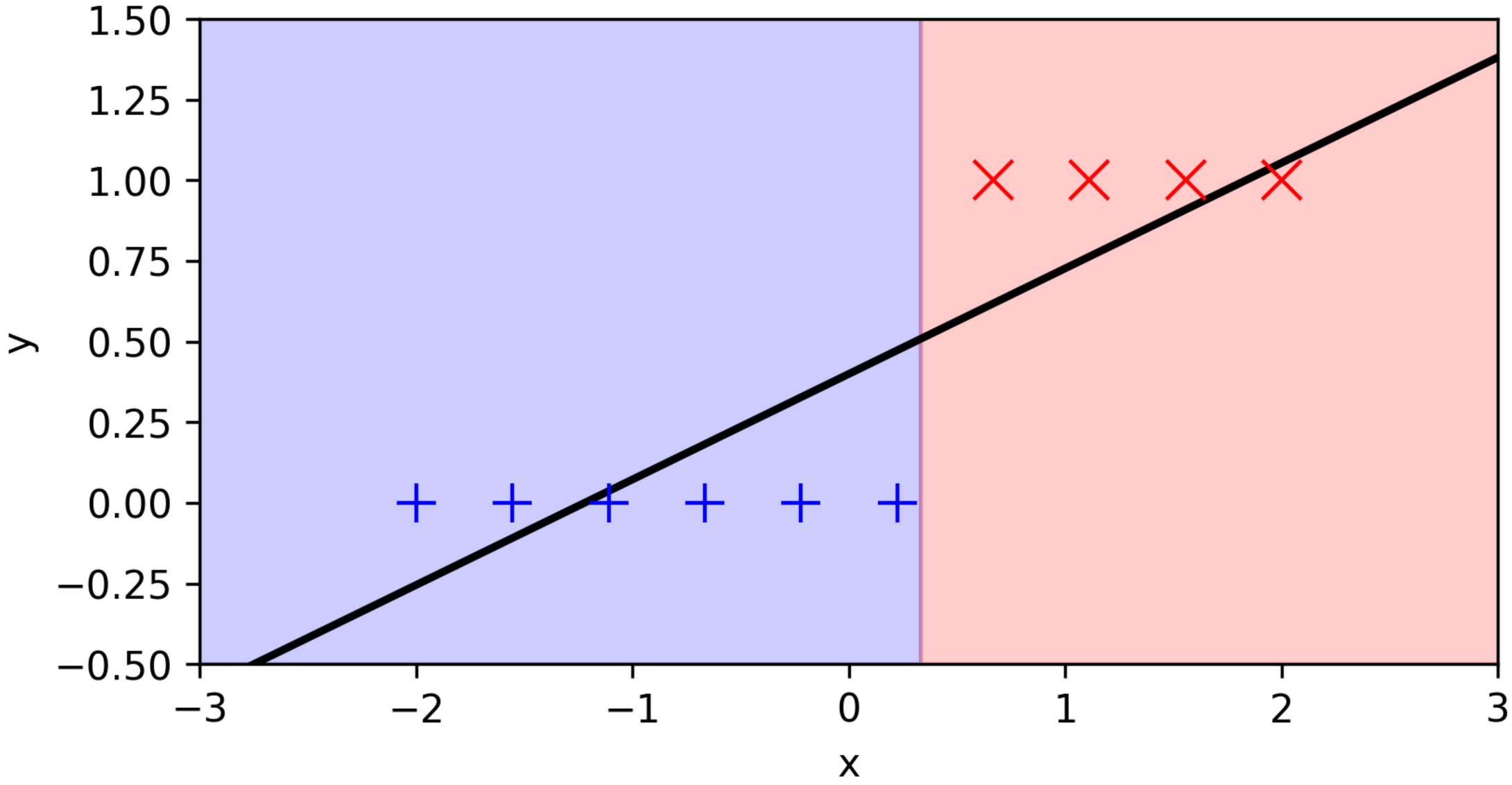

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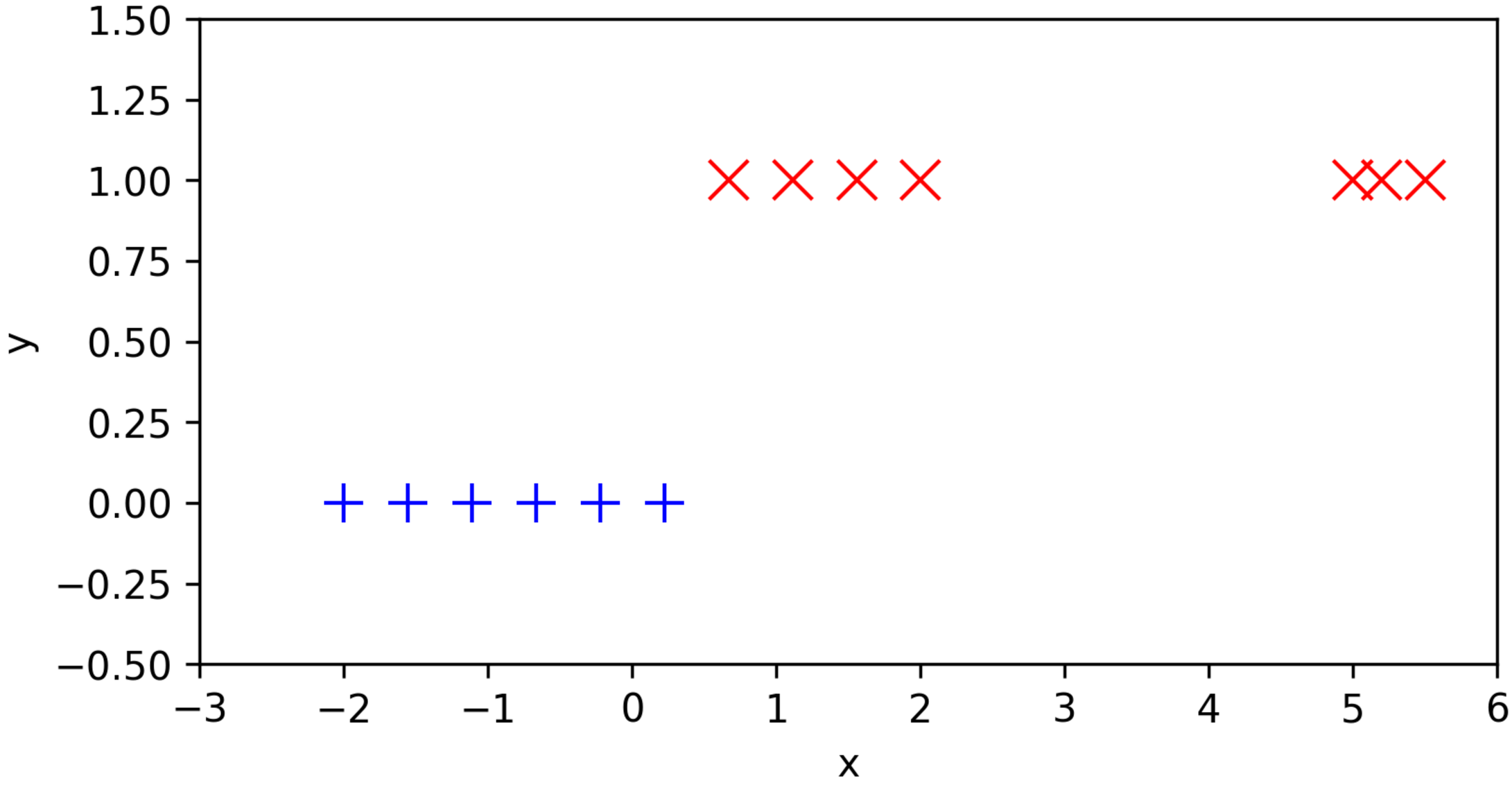

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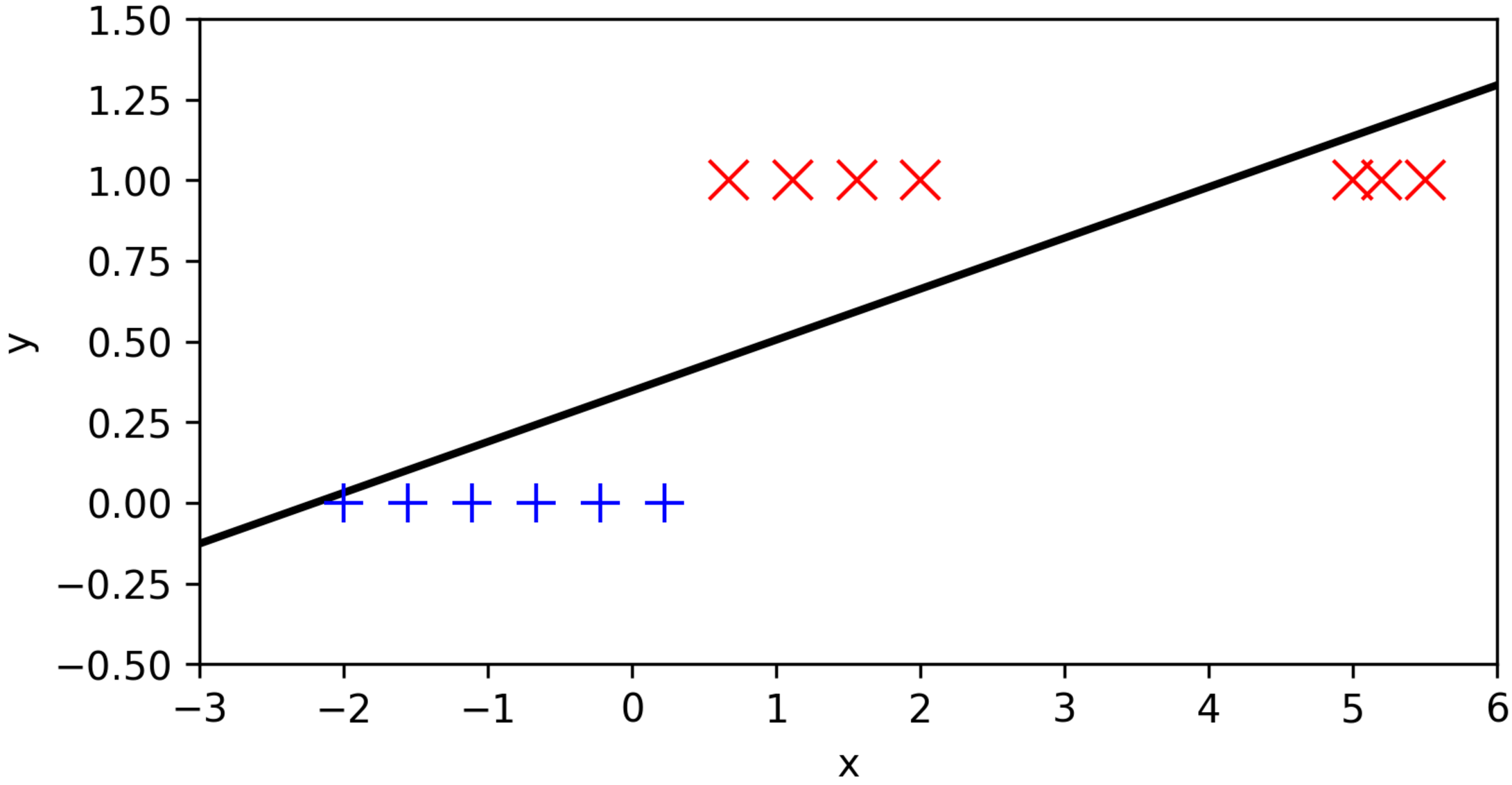

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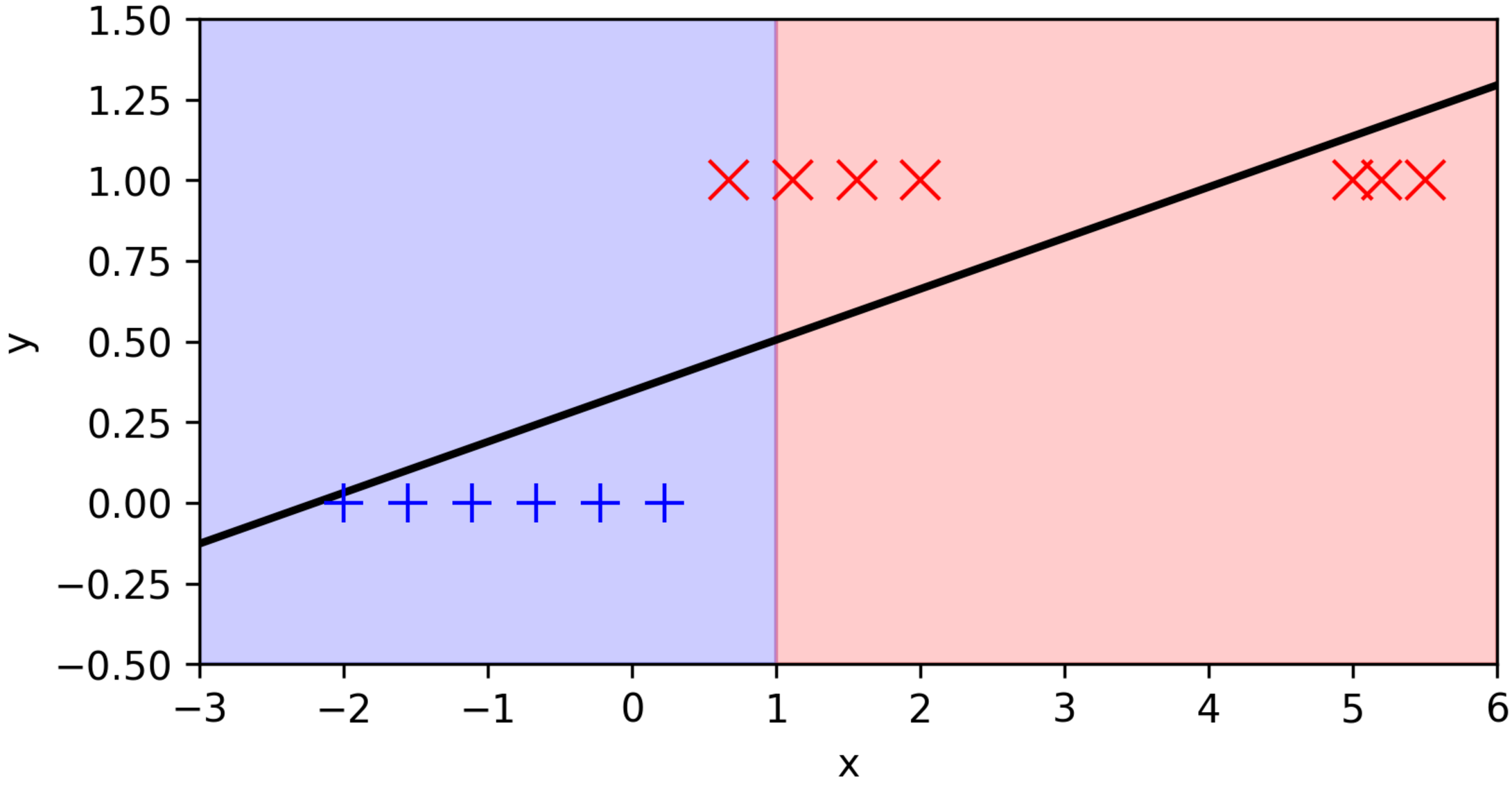

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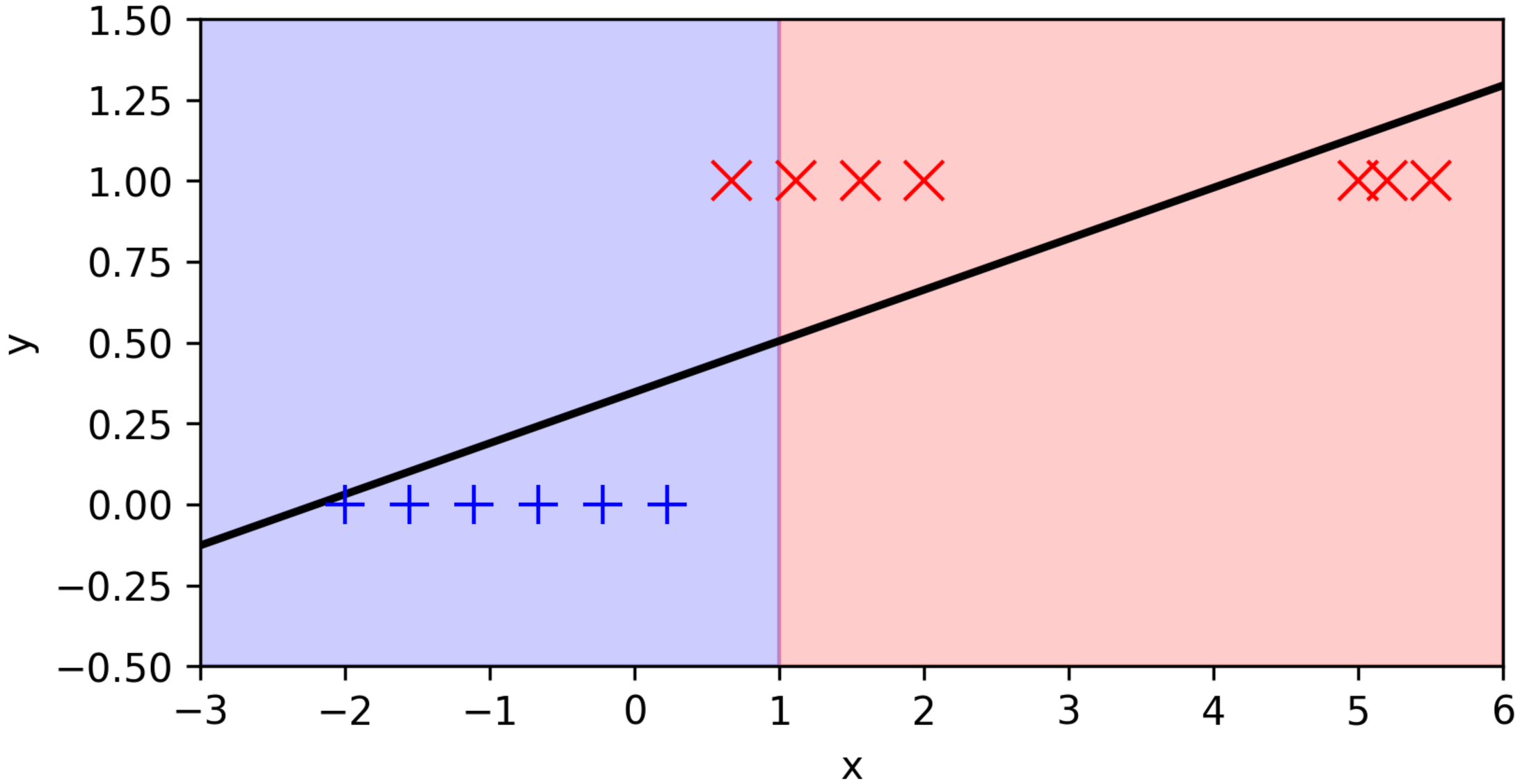

Least squares for classification: Lack robustness. Also fundamentally unsound - remember the Gaussian assumption!

Binary logistic classification - problem set-up

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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

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

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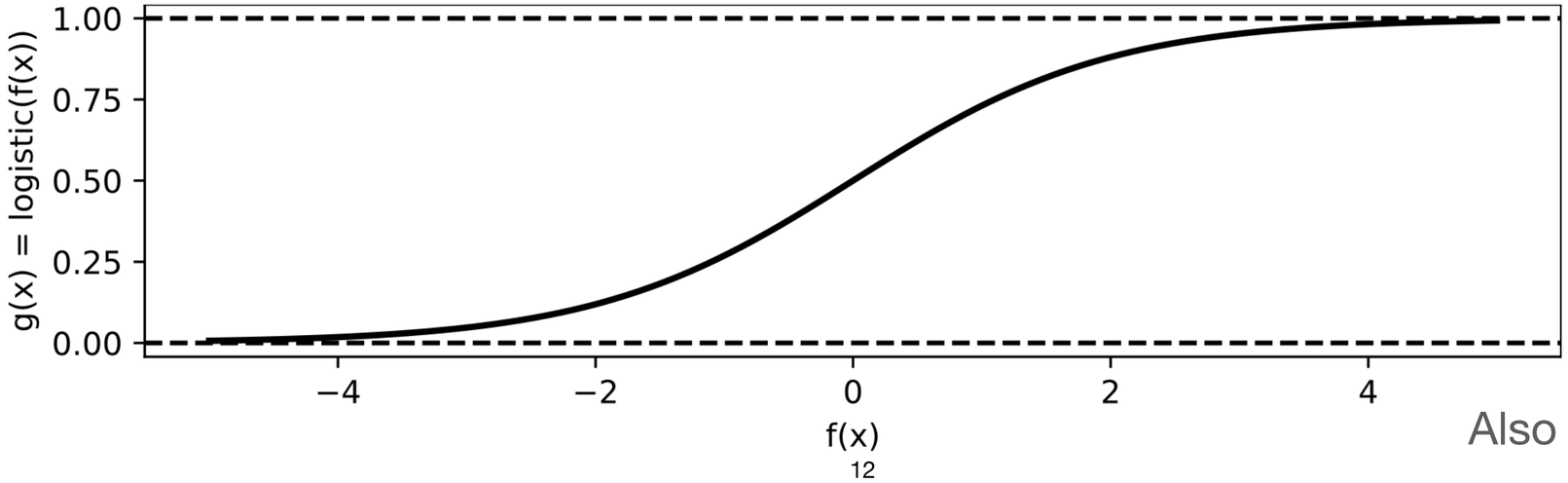
Want: $0 \leq g_\theta(x) \leq 1, \forall x$

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

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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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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* 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:**

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

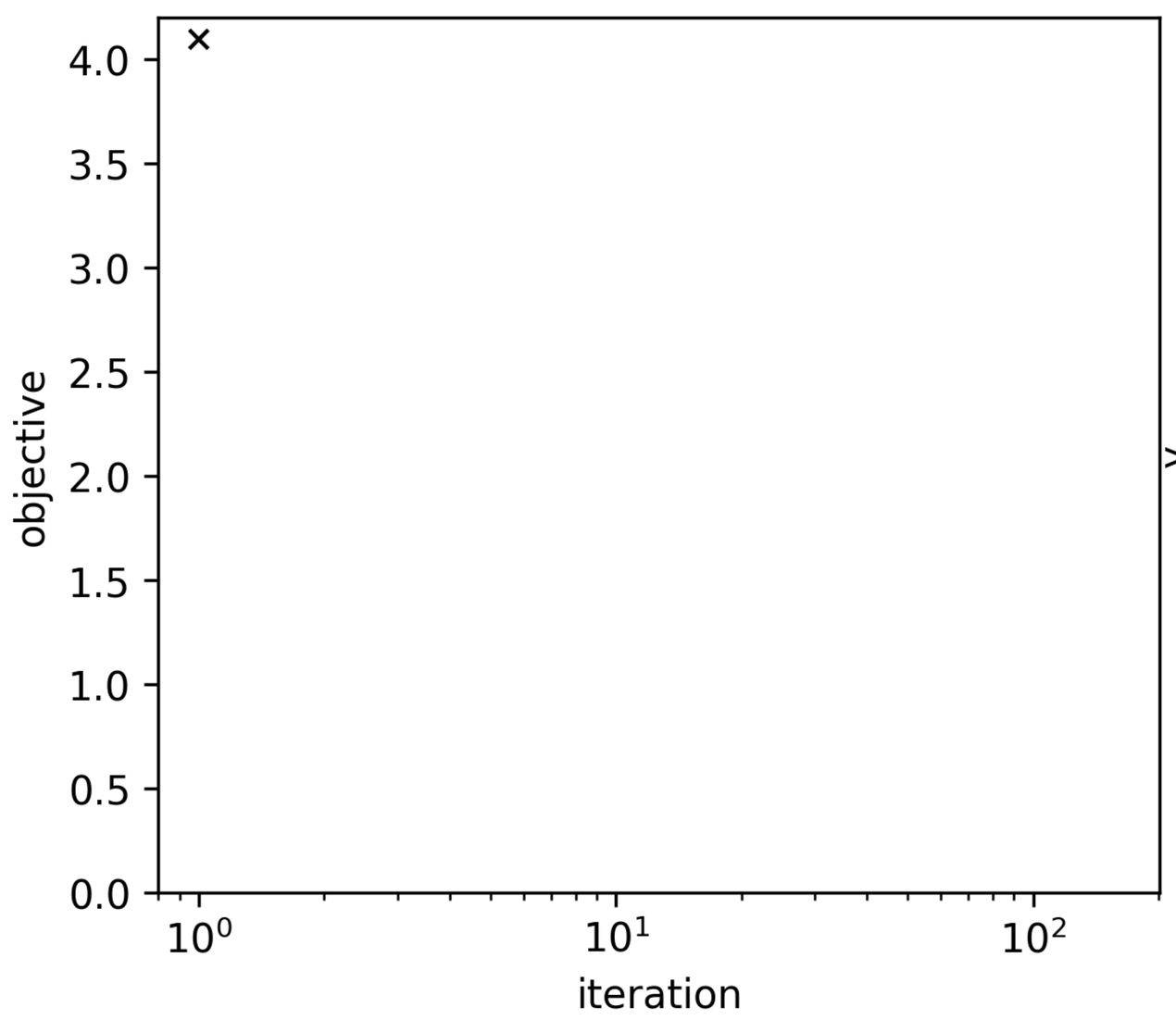
Data-fit
Lower = better fit

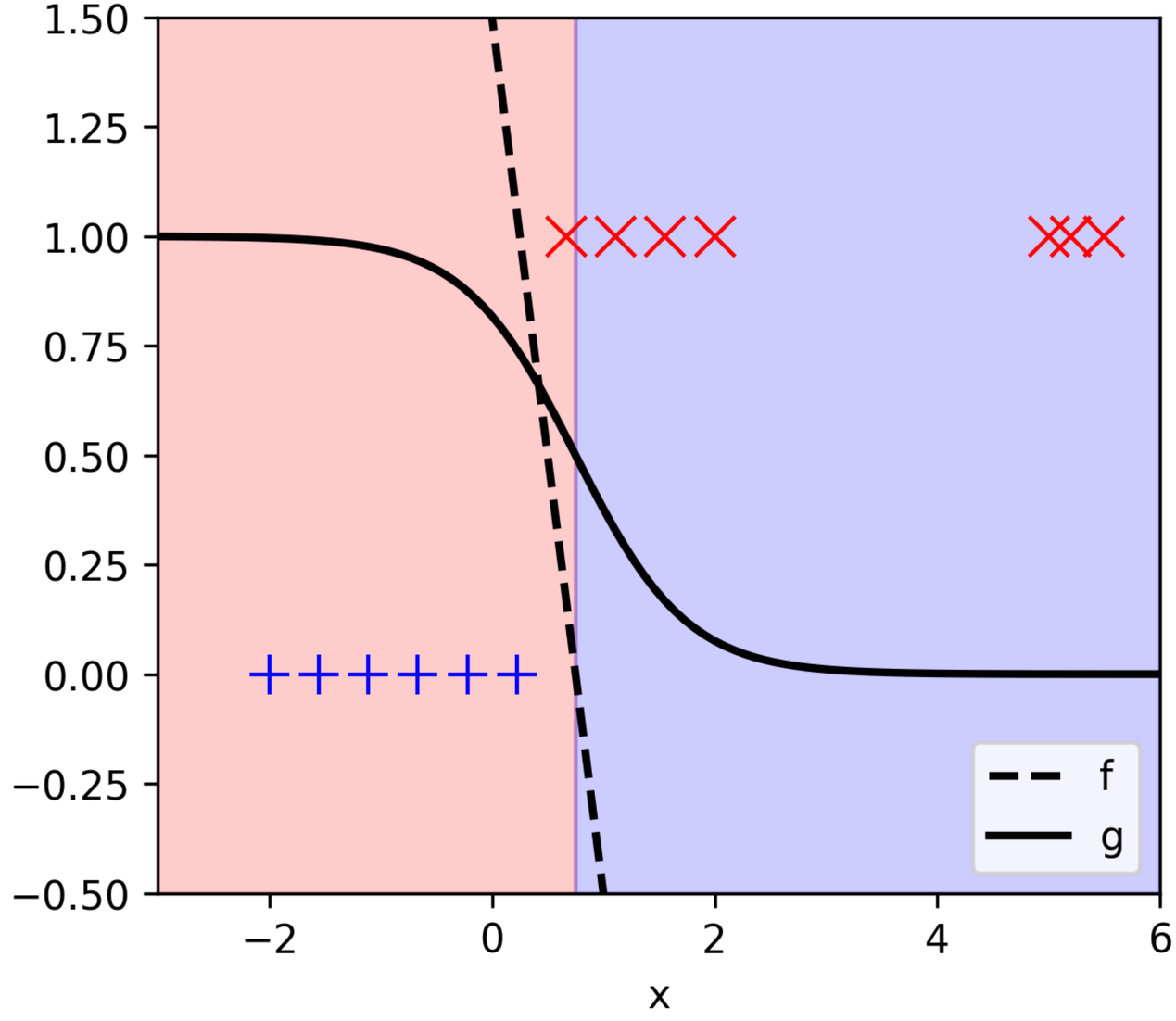
Regulariser
Lower = simpler model

Hyperparameter

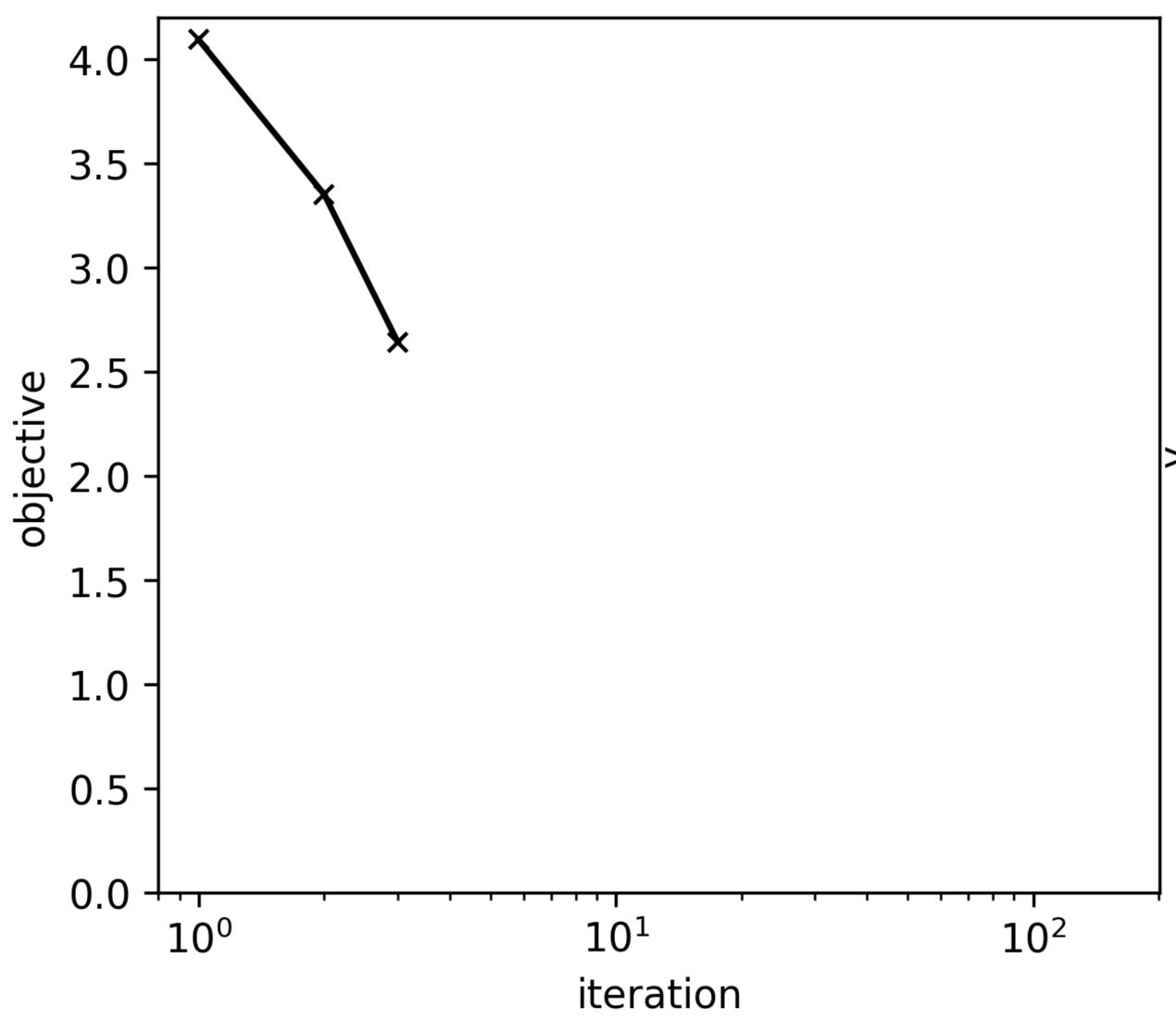
Binary logistic classification - example

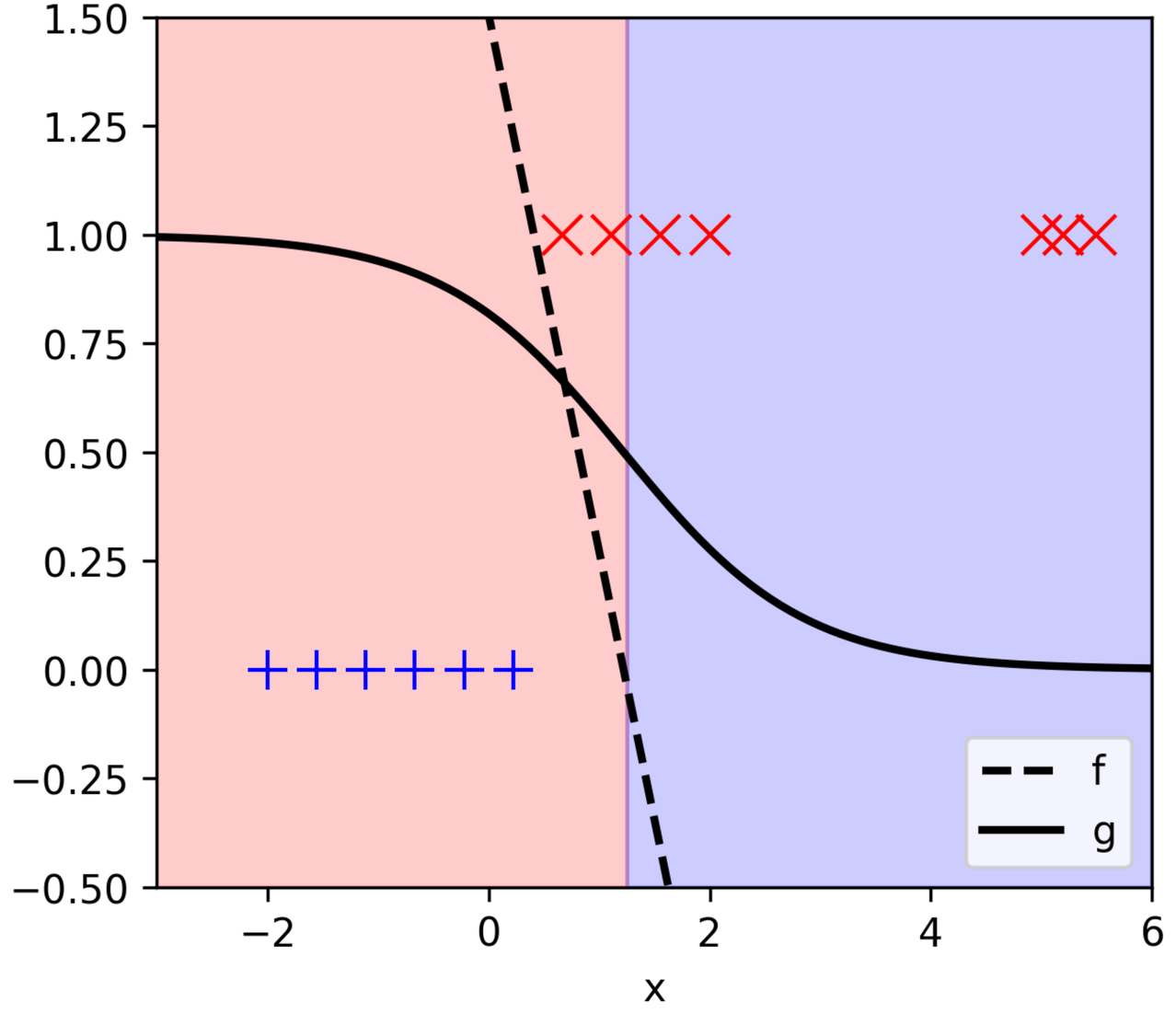
Binary logistic classification - example





Binary logistic classification - example





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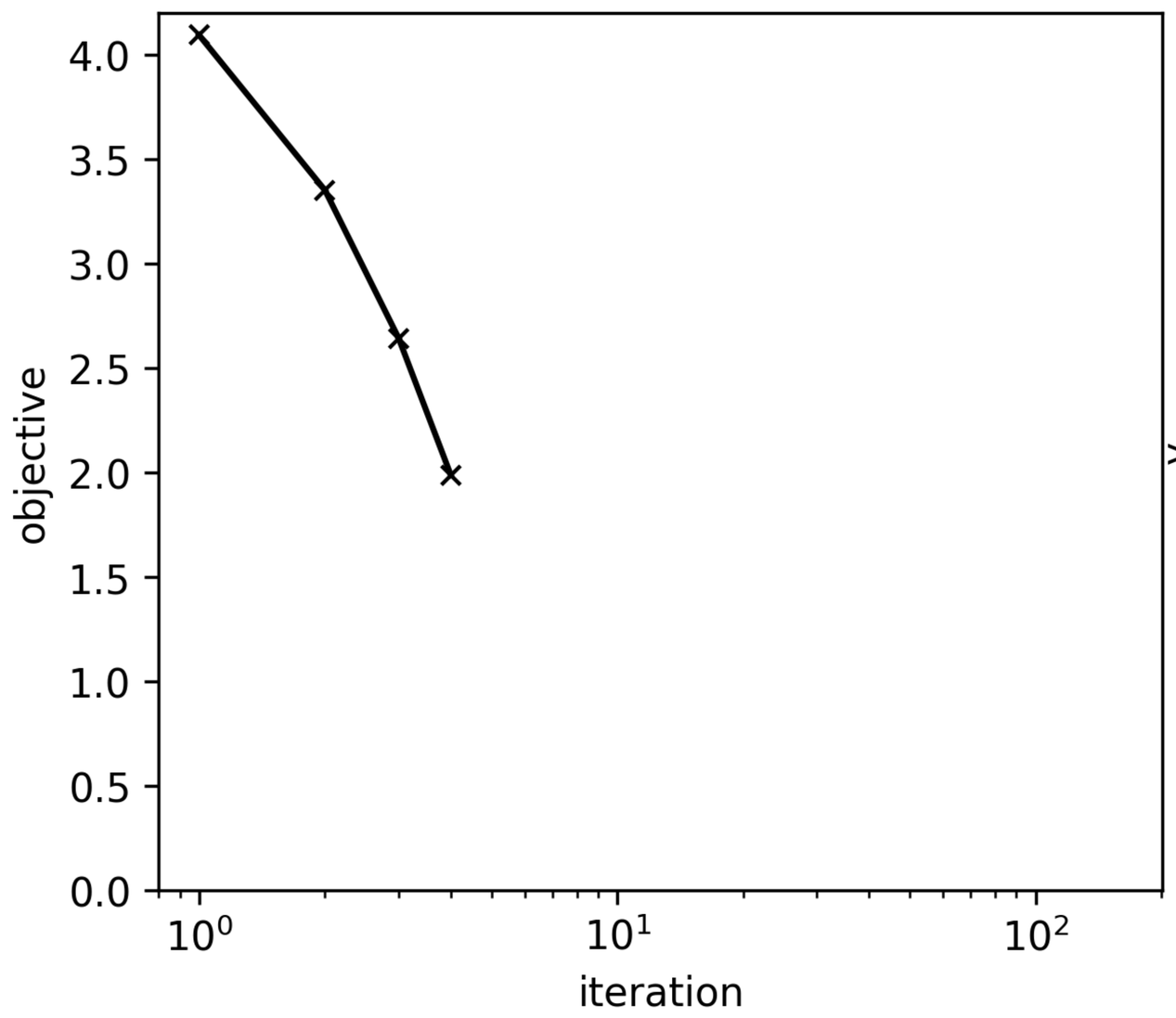

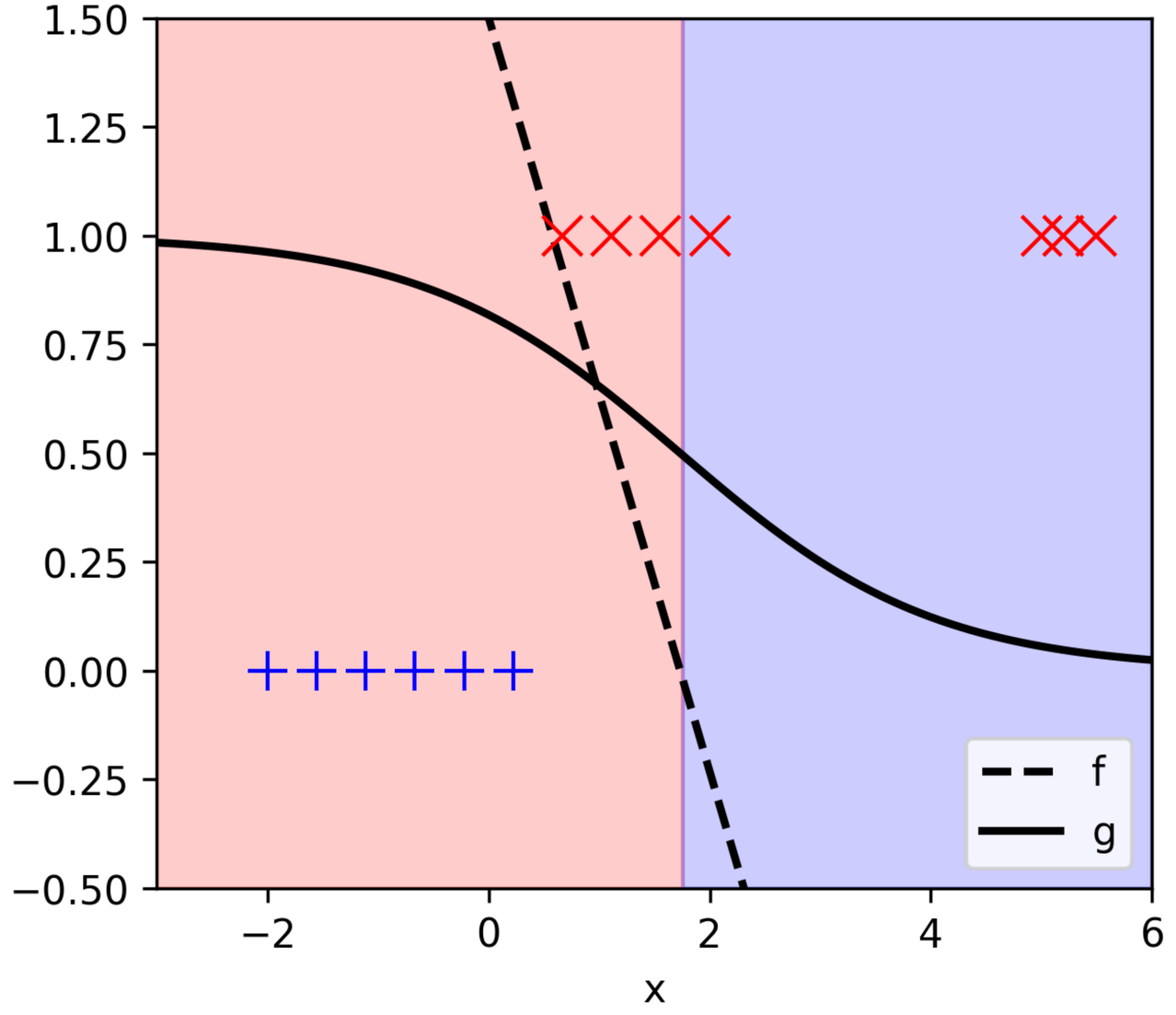

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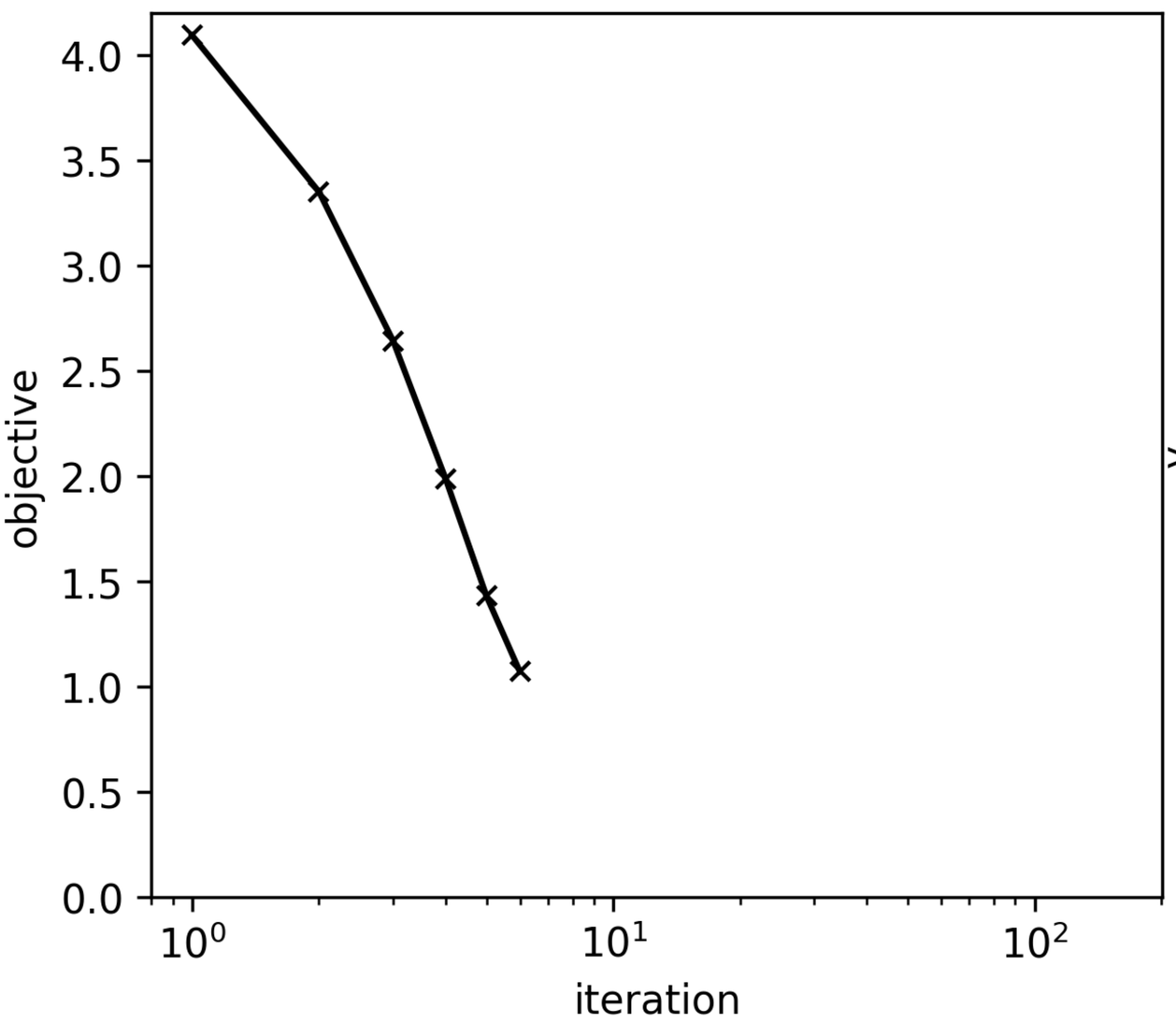

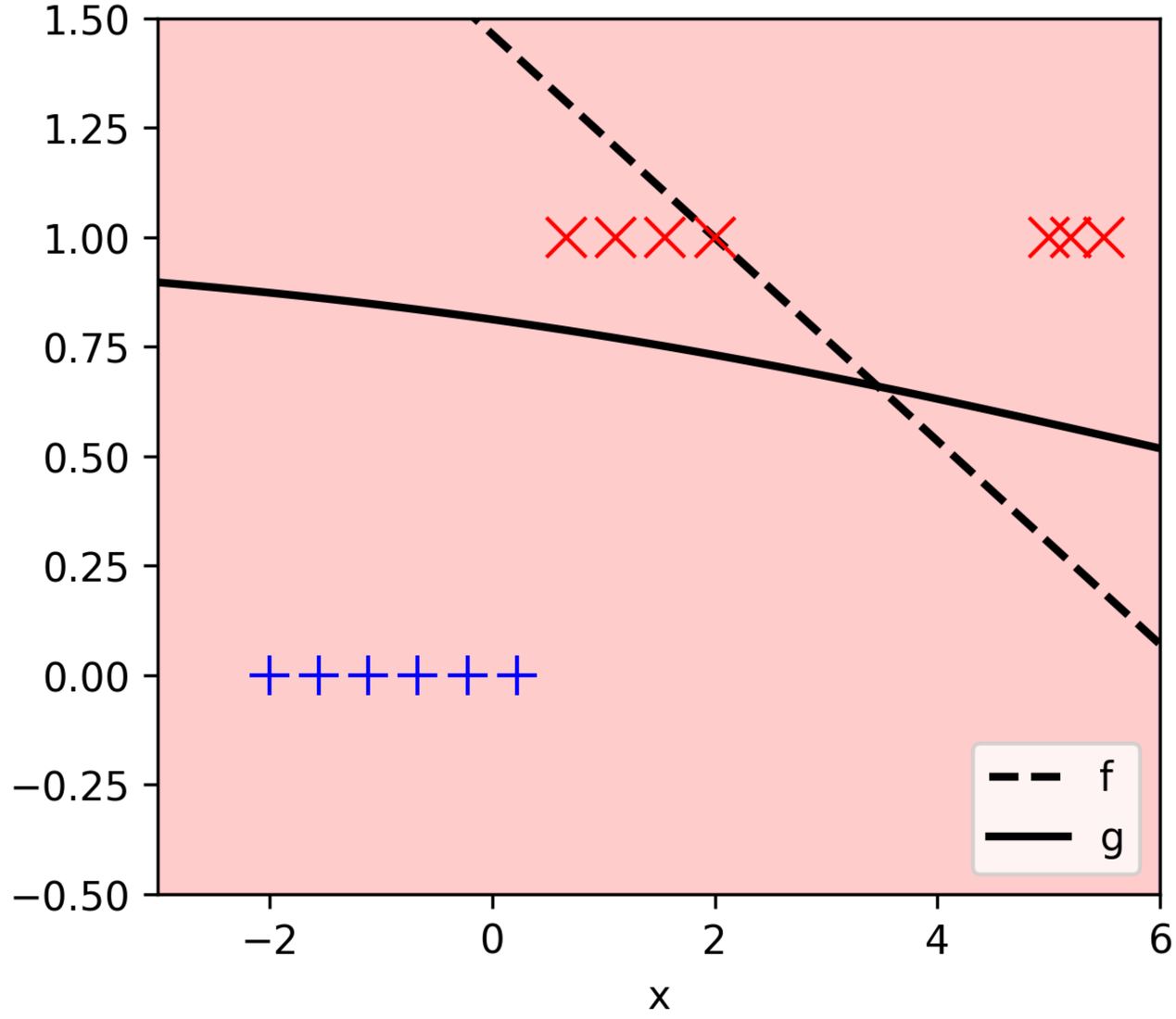

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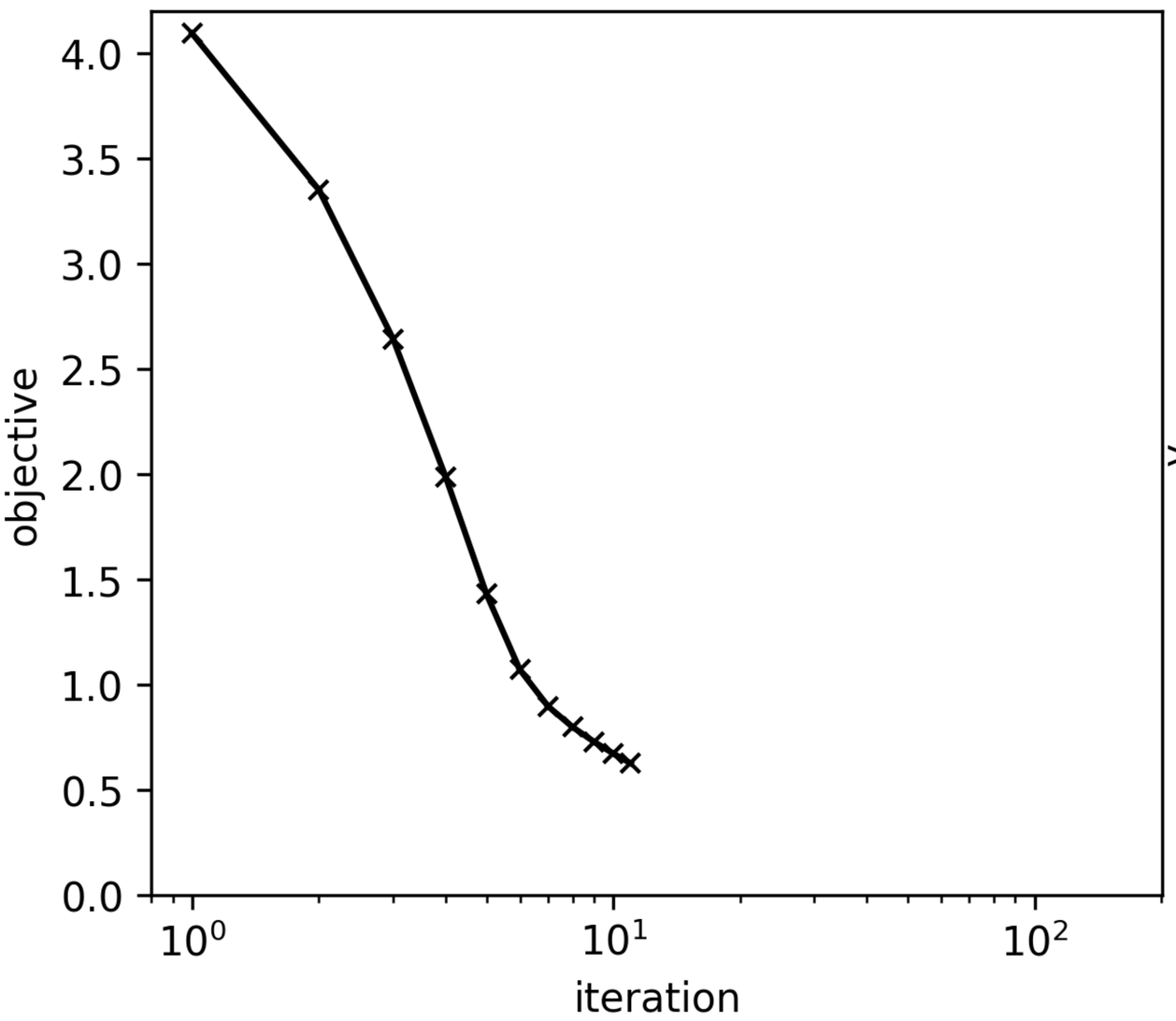

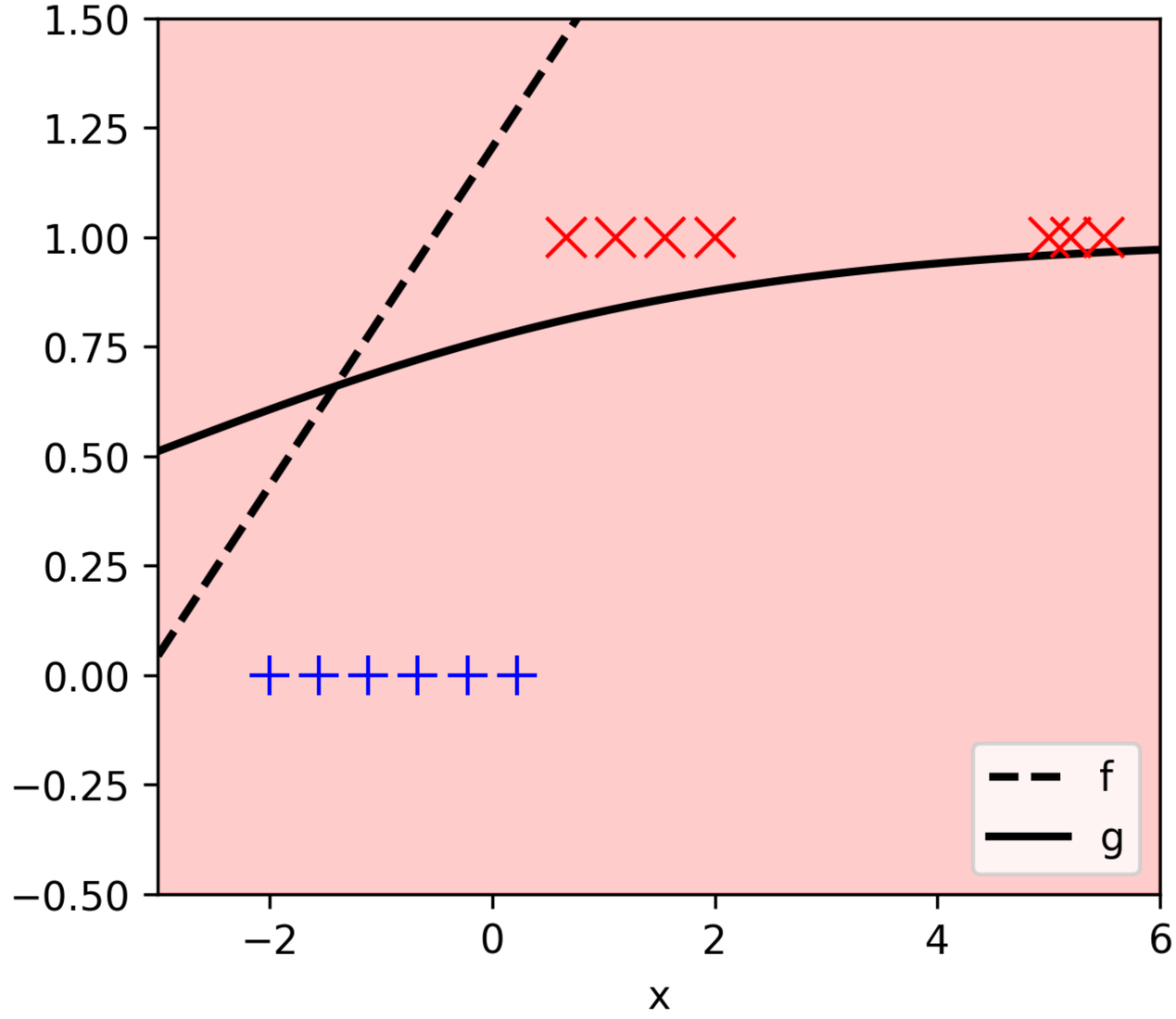

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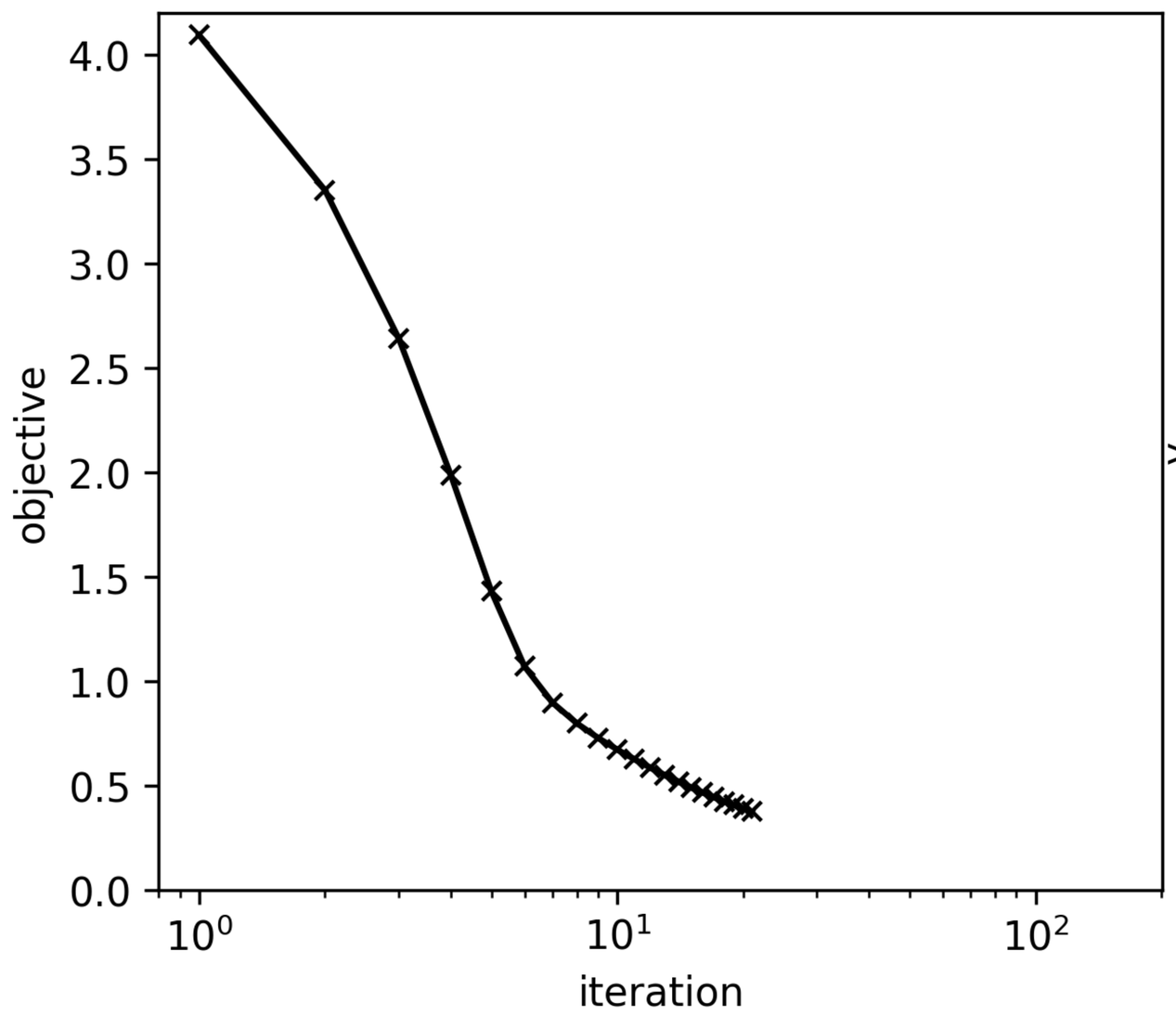

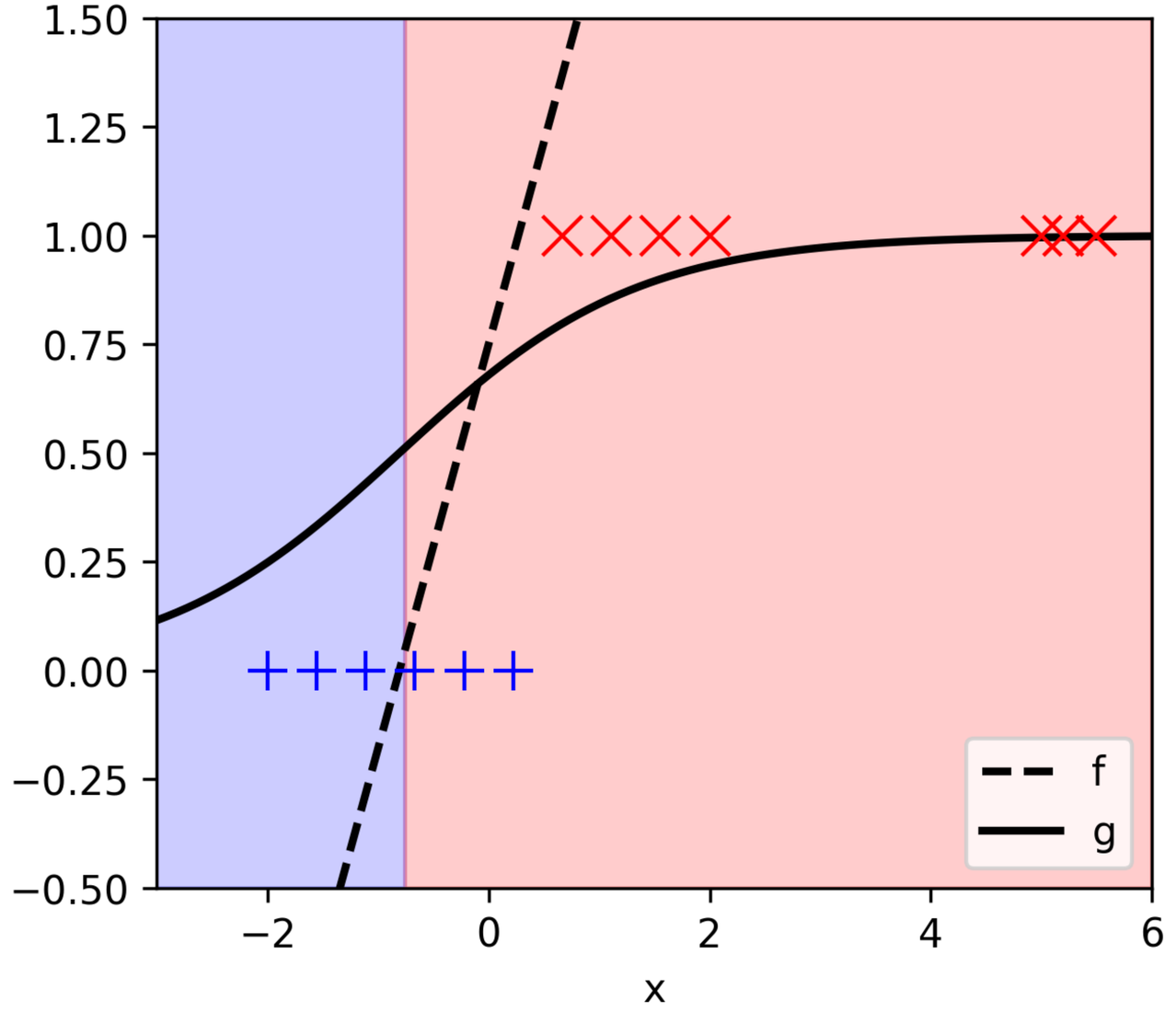

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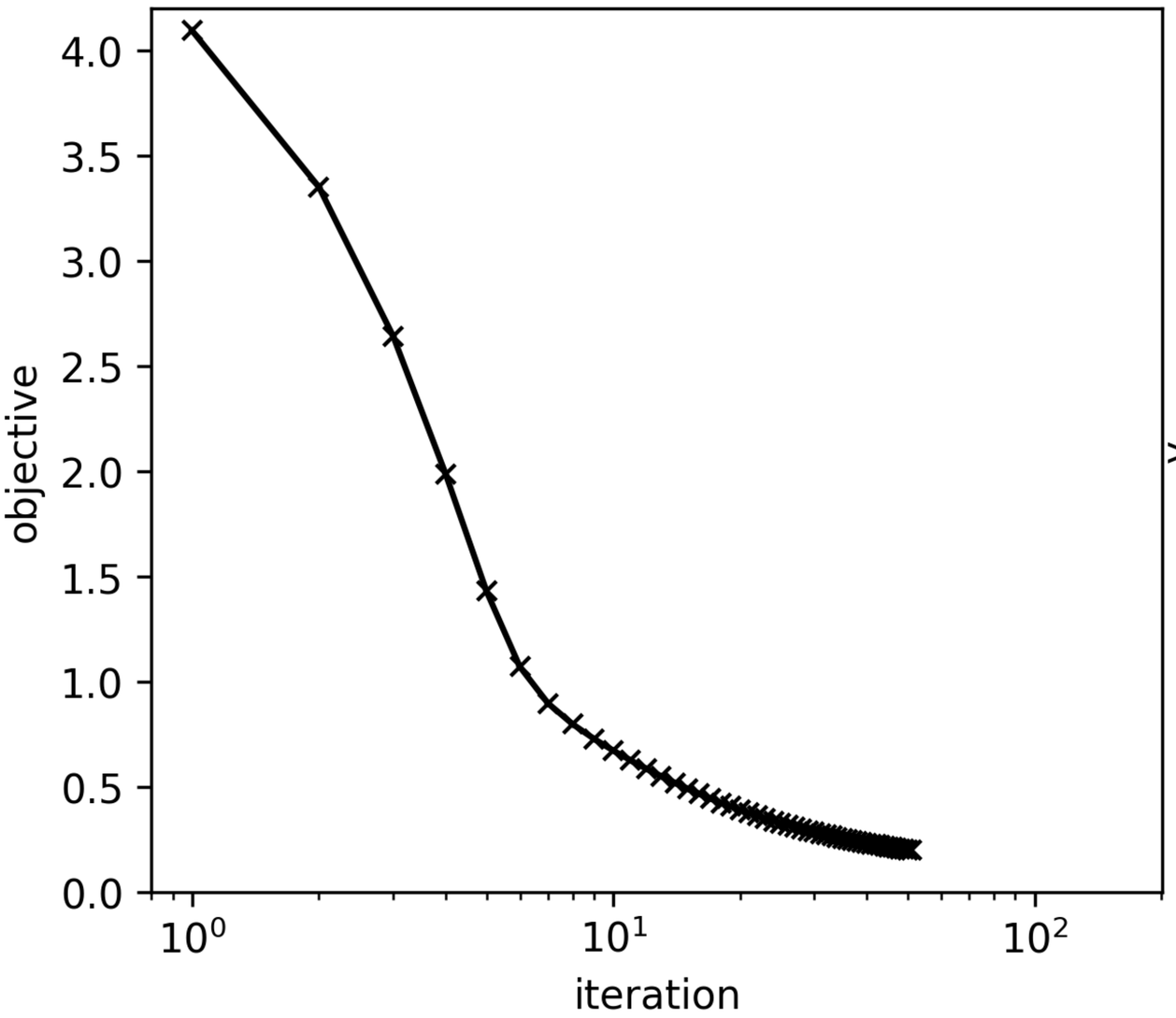

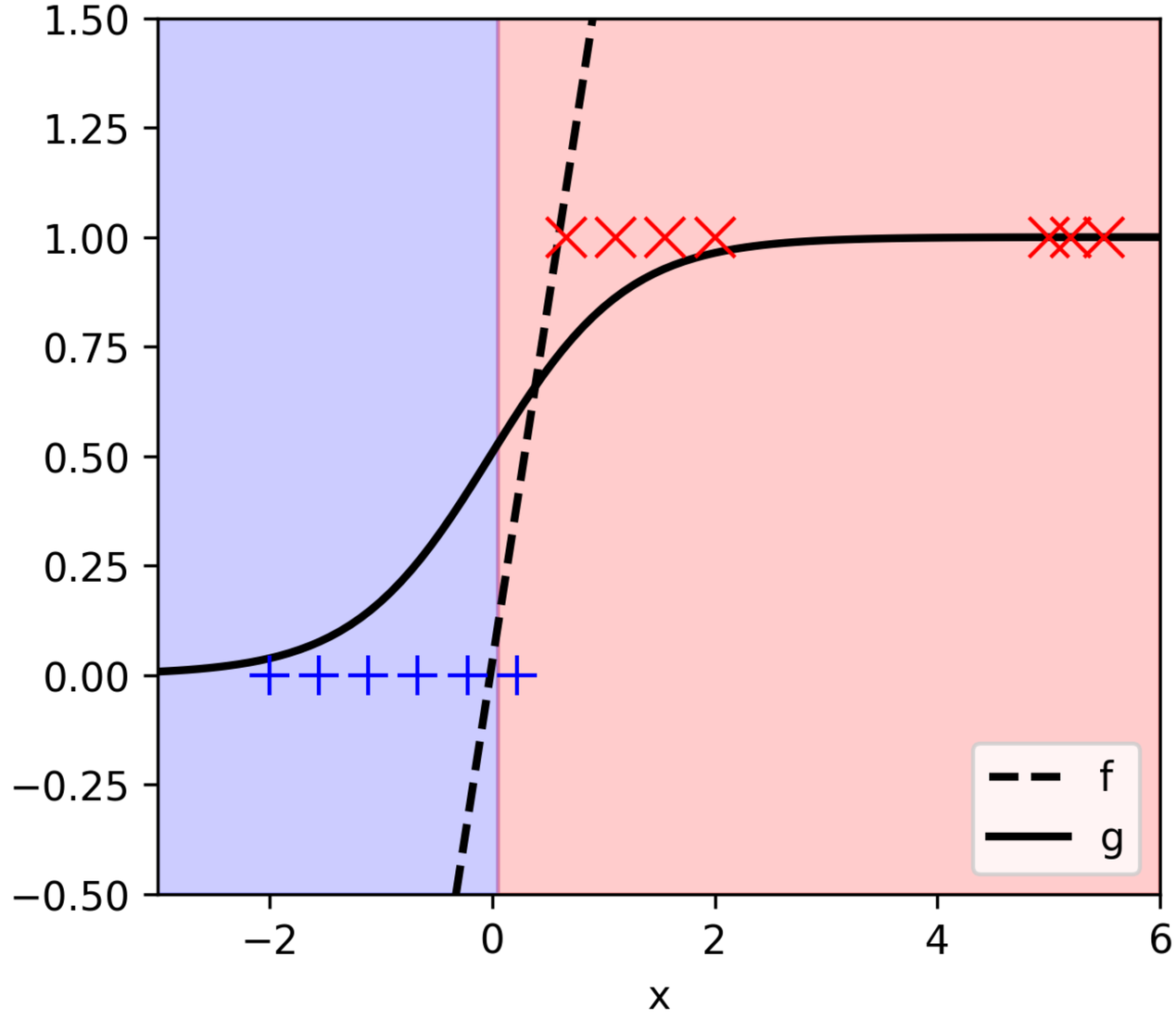

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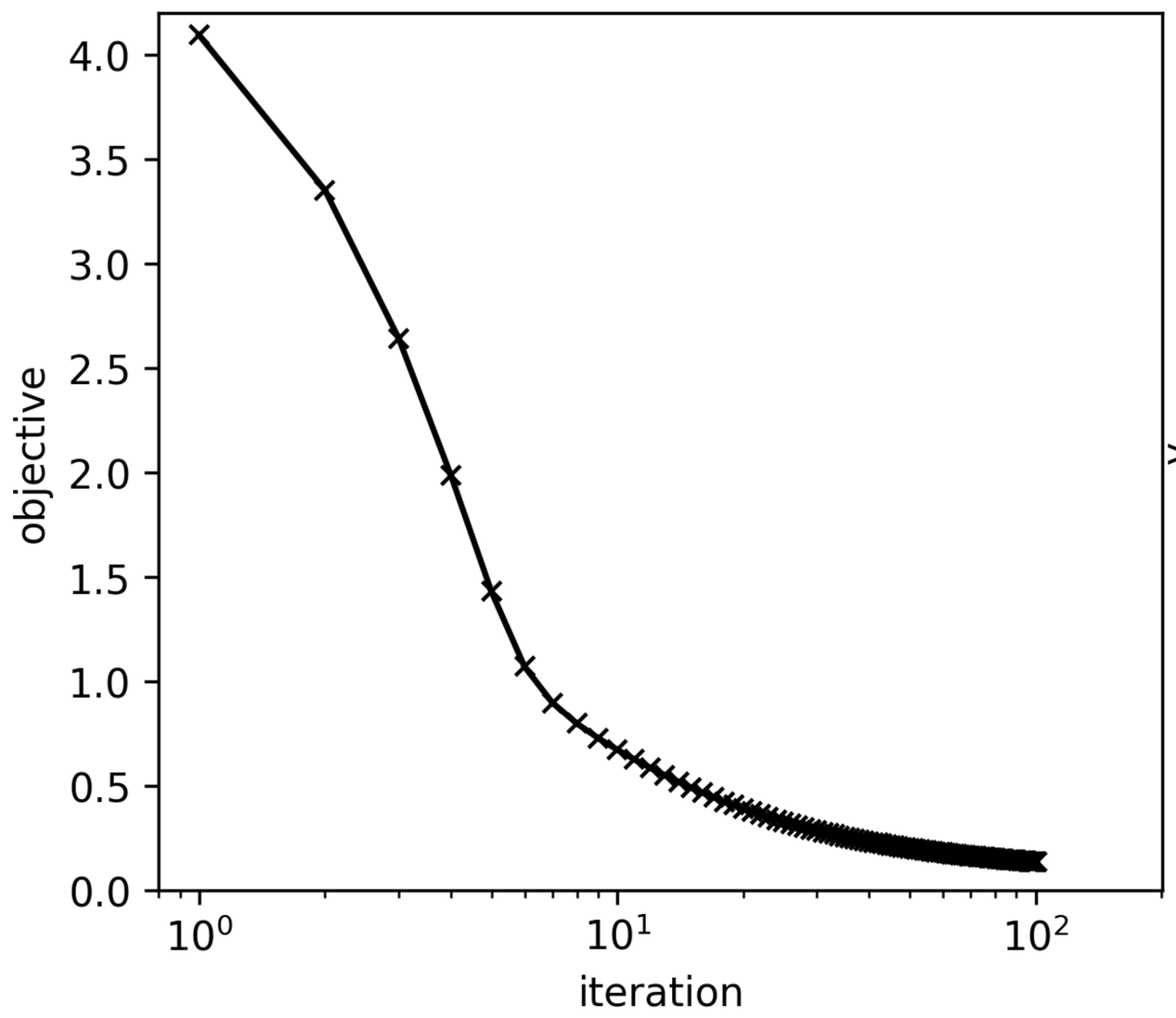

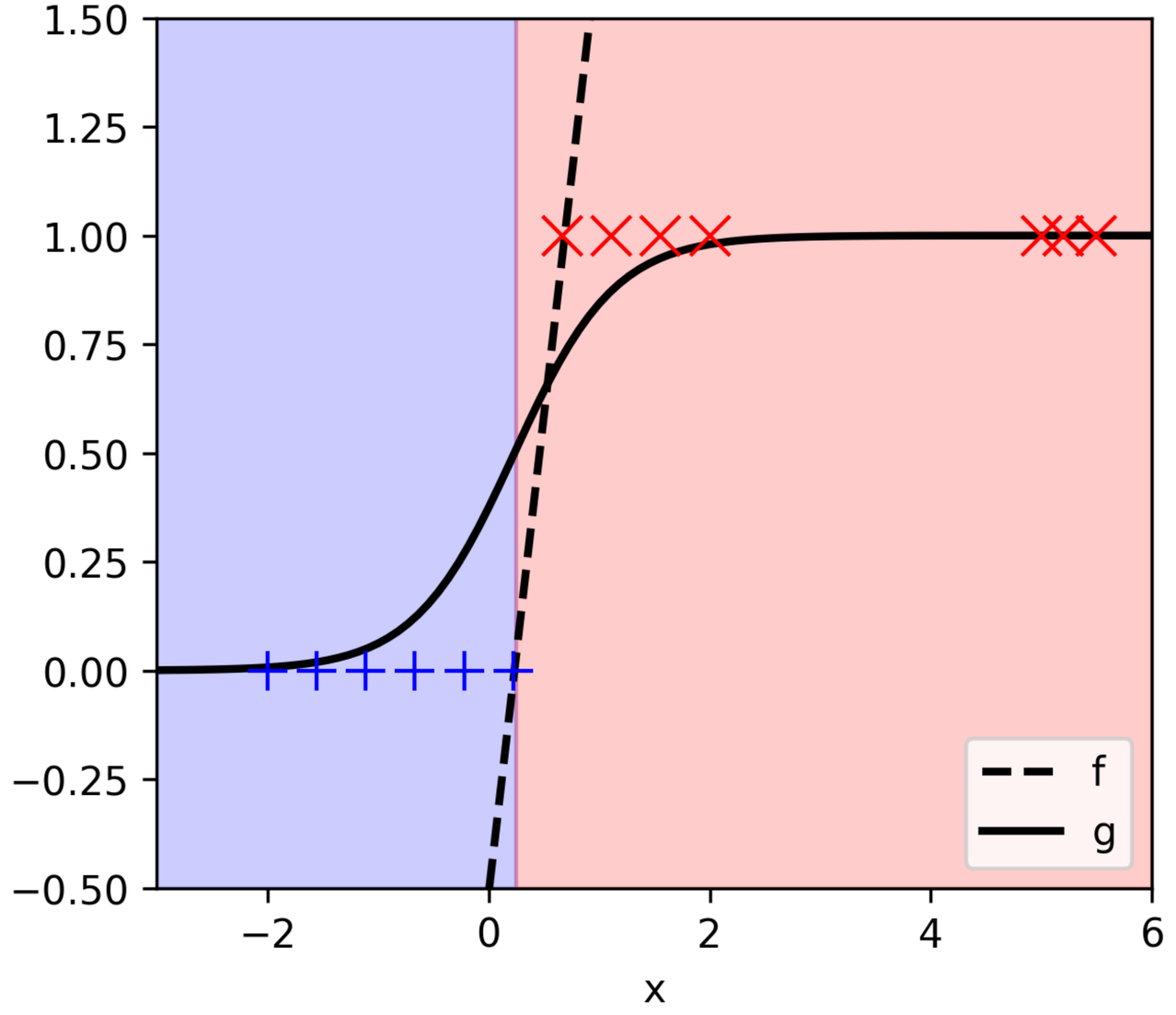

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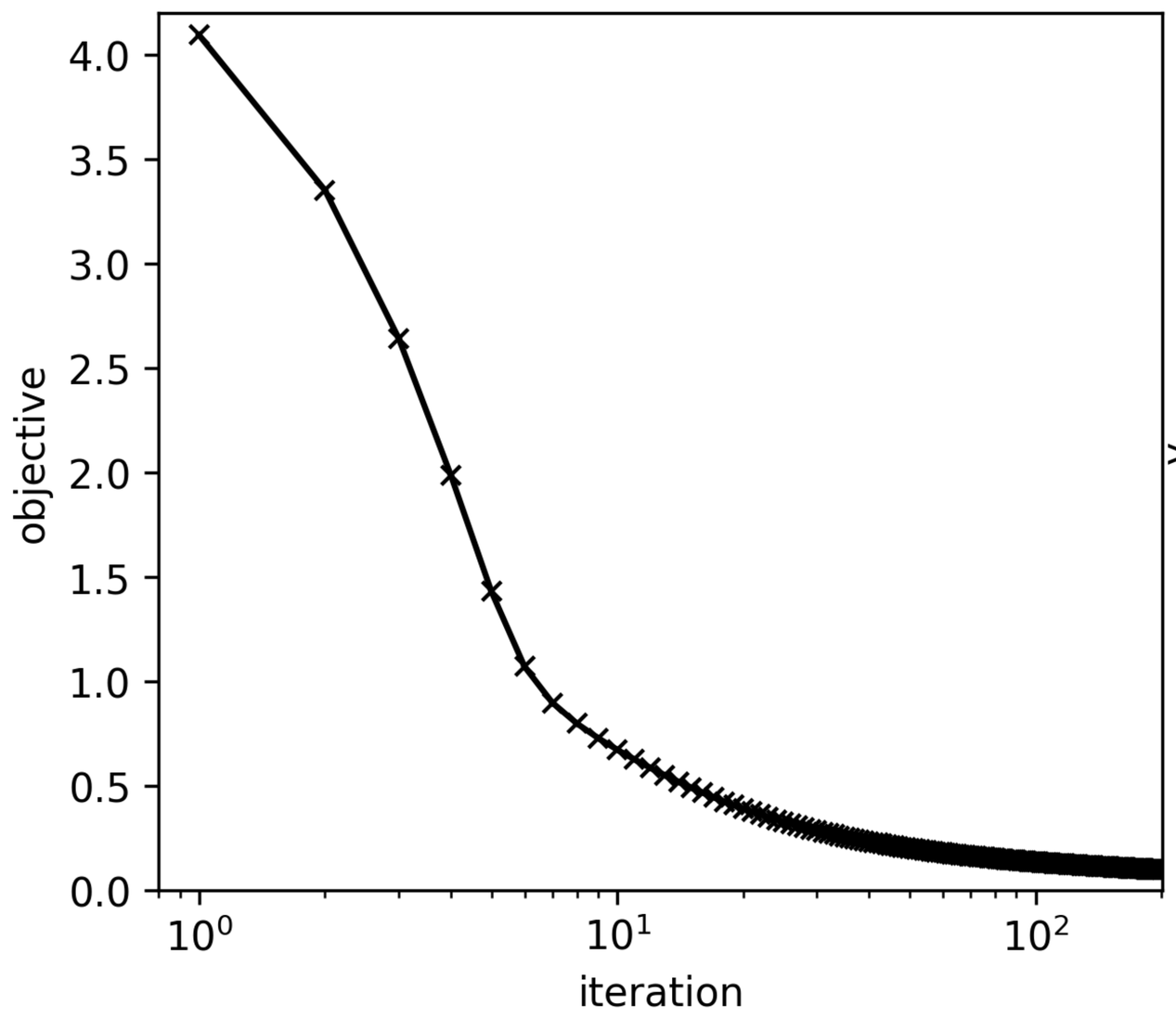

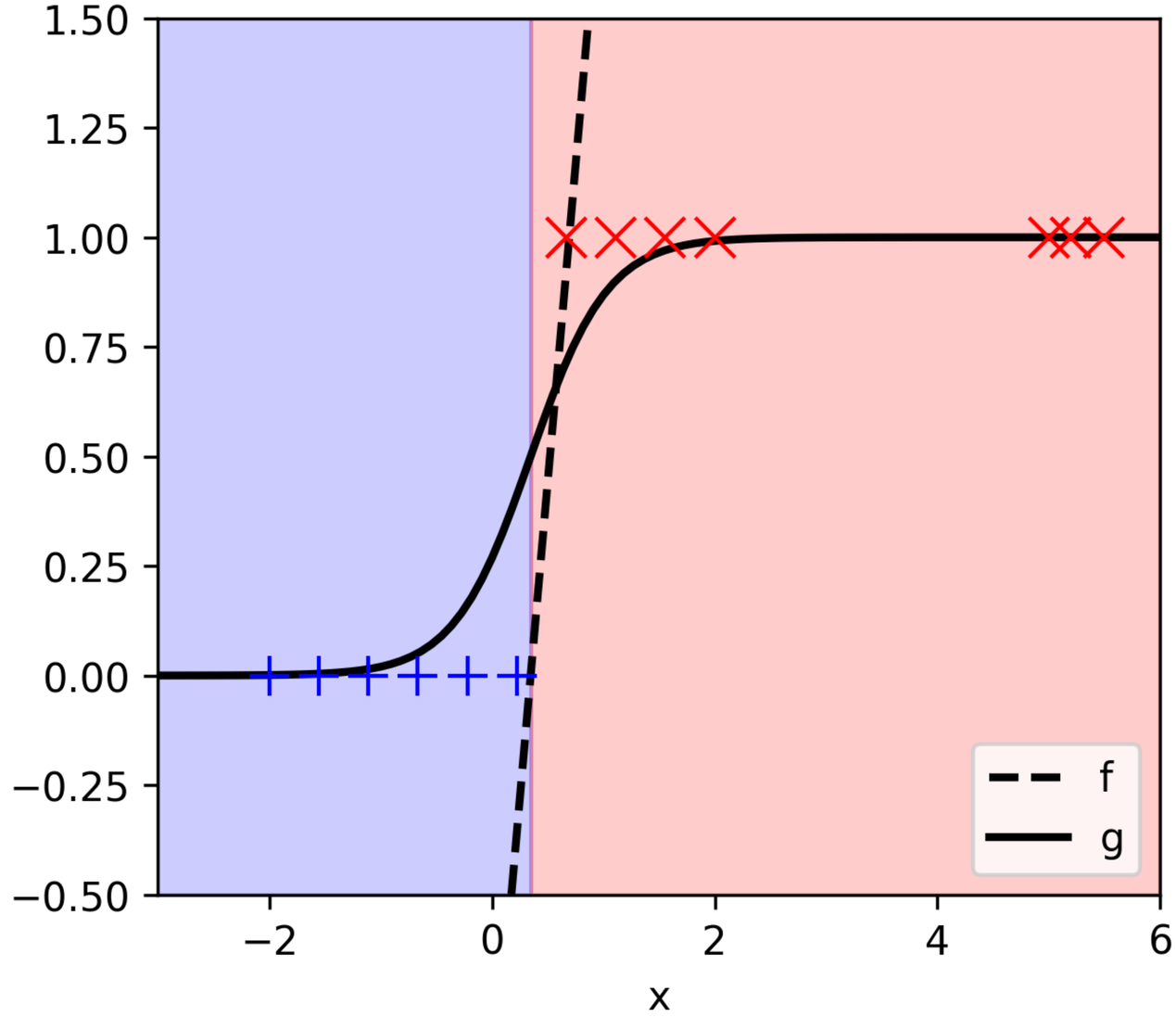

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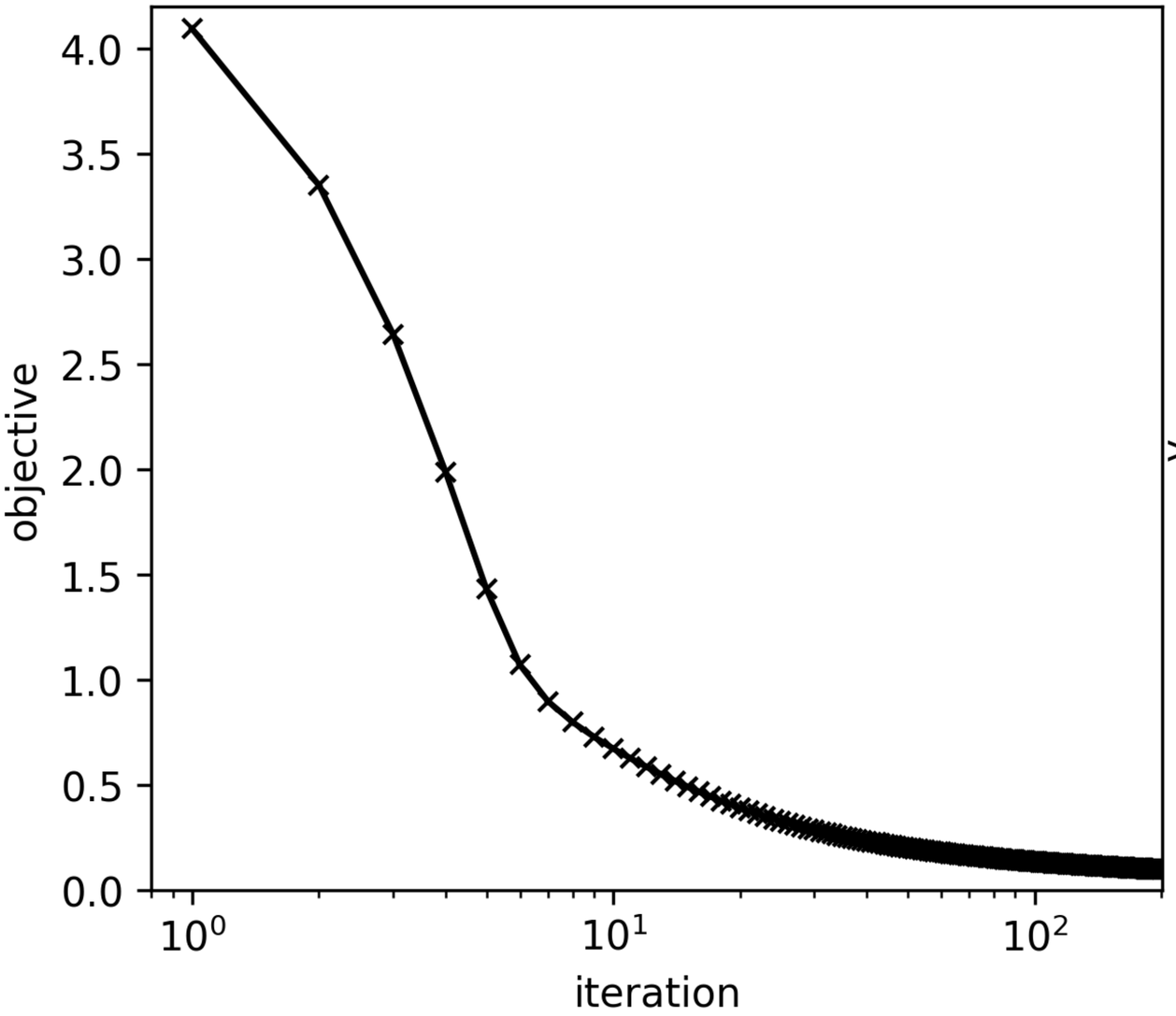

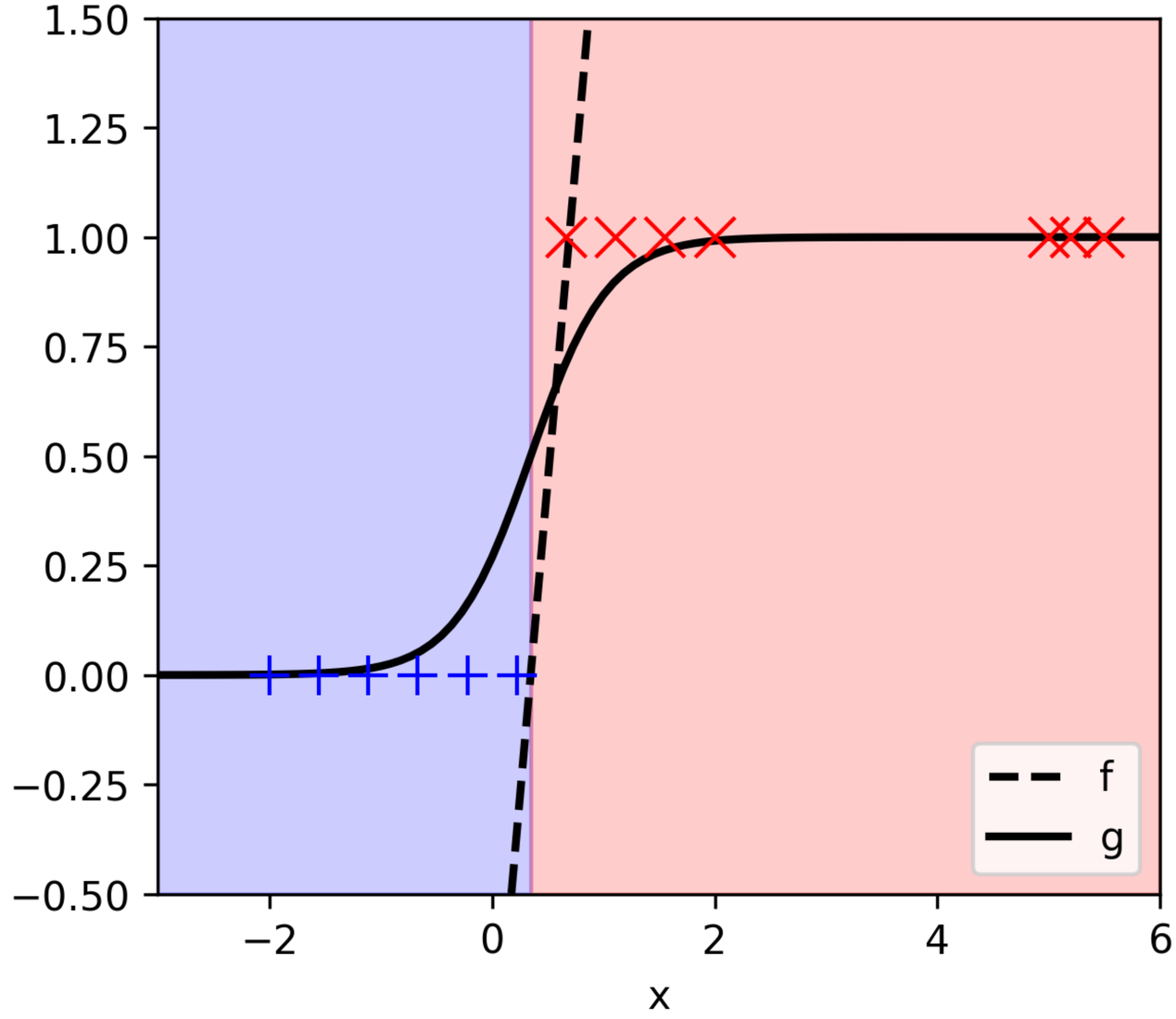

More examples: https://playground.tensorflow.org/

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

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:	$p(\mathscr{D} \mid \theta) = \prod_n \mathcal{N}(y_n; f_\theta(x_n), \sigma^2)$	$p(\mathscr{D} \mid \theta) = \prod_n \text{Bernoulli}(y_n; g_\theta(x_n))$ $g_\theta(x) = \sigma(f_\theta(x))$, σ is logistic sigmoid
Closed form: $\theta = (X^\intercal X + \lambda \mathrm{I})^{-1} X^\intercal \mathbf{y}$ or $\theta = (X^\intercal X)^{-1} X^\intercal \mathbf{y}$		✗

Have to use numerical optimisation

Overview

1. Recap: Linear regression
2. Discriminative: From least squares to binary logistic classification
3. **Discriminative: From binary to multi-class classification**
4. Generative model: linear discriminant analysis
5. [Optional] Evaluation
6. [Optional] 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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Training data $\mathscr{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}, \mathbf{x}_n \in \mathbb{R}^D,\ y_n \in \{0,1\}$

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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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Constraints: $0 \leq g_\theta^{(c)}(x) \leq 1, \forall x, c,$ and $\sum_c g_\theta^{(c)}(x) = 1$

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

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

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minimise negative log-likelihood

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

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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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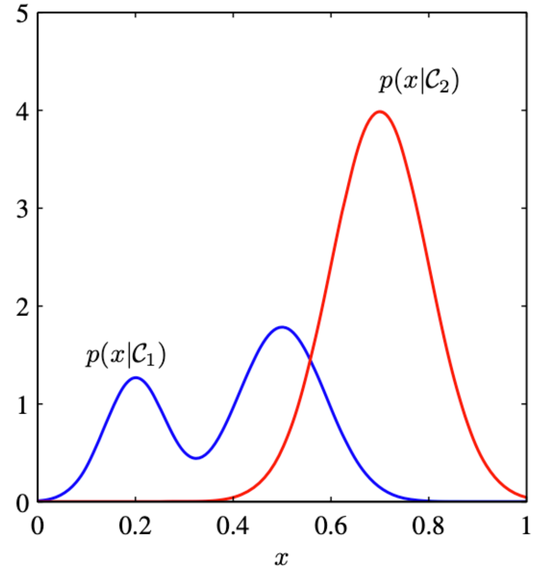
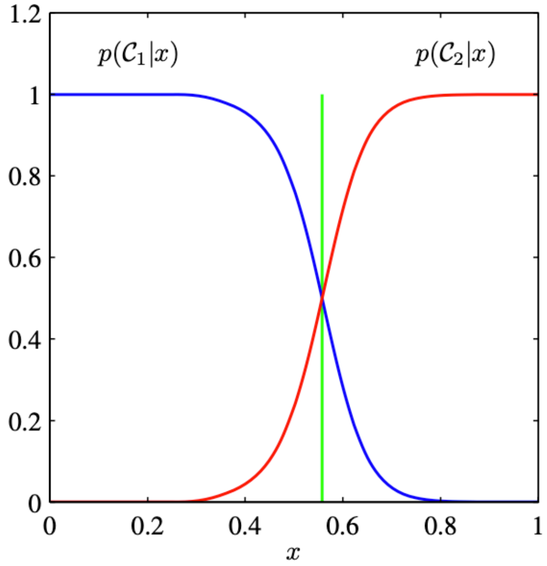
Generative vs discriminative approaches to classification





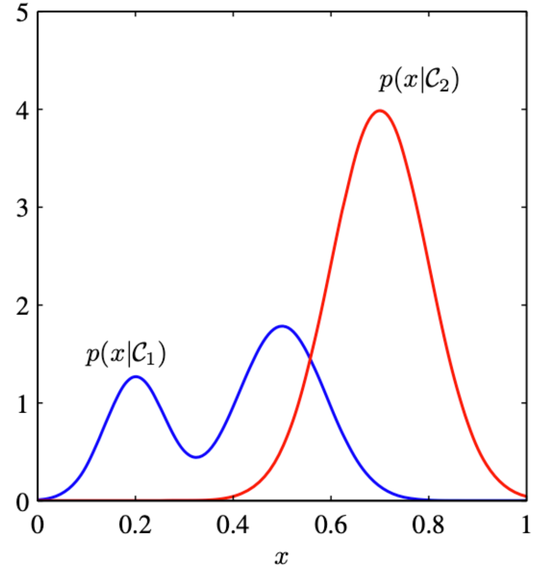
Binary case

Discriminative

$$p_\theta(y \mid \mathbf{x})$$

$$p_\theta(C_1 \mid \mathbf{x}) = g_\theta(\mathbf{x}) = \sigma(f_\theta(\mathbf{x}))$$

Generative vs discriminative approaches to classification



Generative

$$p_\theta(\mathbf{x}, y) = p_\theta(\mathbf{x} \mid y) p_\theta(y)$$

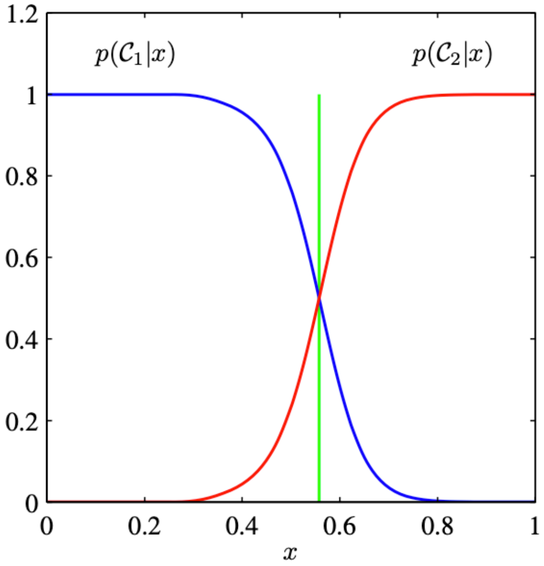
Binary case

Denote y = 1 as C_1 and y = 0 as C_0

$$p_\theta(C_1 \mid \mathbf{x}) = \frac{p_\theta(\mathbf{x}, C_1)}{p_\theta(\mathbf{x}, C_1) + p_\theta(\mathbf{x}, C_0)}$$

$$= \frac{p_\theta(\mathbf{x} \mid C_1) p_\theta(C_1)}{p_\theta(\mathbf{x} \mid C_1) p_\theta(C_1) + p_\theta(\mathbf{x} \mid C_0) p_\theta(C_0)}$$

$$= \frac{1}{1 + \exp(-a)} = \sigma(a) \quad \text{where} \quad a = \ln \frac{p_\theta(\mathbf{x} \mid C_1) p_\theta(C_1)}{p_\theta(\mathbf{x} \mid C_0) p_\theta(C_0)}$$



Discriminative

$$p_\theta(y \mid \mathbf{x})$$

$$p_\theta(C_1 \mid \mathbf{x}) = g_\theta(\mathbf{x}) = \sigma(f_\theta(\mathbf{x}))$$

A Generative example: Linear discriminant analysis

Denote y = 1 as C_1 and y = 0 as C_0

$$p_\theta(C_1 \mid \mathbf{x}) = \frac{p_\theta(x, C_1)}{p_\theta(\mathbf{x}, C_1) + p_\theta(\mathbf{x}, C_0)} = \frac{p_\theta(\mathbf{x} \mid C_1)p_\theta(C_1)}{p_\theta(\mathbf{x} \mid C_1)p_\theta(C_1) + p_\theta(\mathbf{x} \mid C_0)p_\theta(C_0)} = \frac{1}{1 + \exp(-a)} = \sigma(a) \quad \text{where} \quad a = \ln \frac{p_\theta(\mathbf{x} \mid C_1)p_\theta(C_1)}{p_\theta(\mathbf{x} \mid C_0)p_\theta(C_0)}$$

Model:

$$p_\theta(\mathbf{x} \mid C_1) = \mathcal{N}(\mathbf{x}; \mu_1, \Sigma) = (2\pi)^{-\frac{D}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_1)^T \Sigma^{-1} (\mathbf{x} - \mu_1)\right)$$

$$p_\theta(\mathbf{x} \mid C_2) = \mathcal{N}(\mathbf{x}; \mu_2, \Sigma) = (2\pi)^{-\frac{D}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_2)^T \Sigma^{-1} (\mathbf{x} - \mu_2)\right)$$

$$p_\theta(C_1) = \pi_1, \quad p_\theta(C_2) = 1 - \pi_1$$

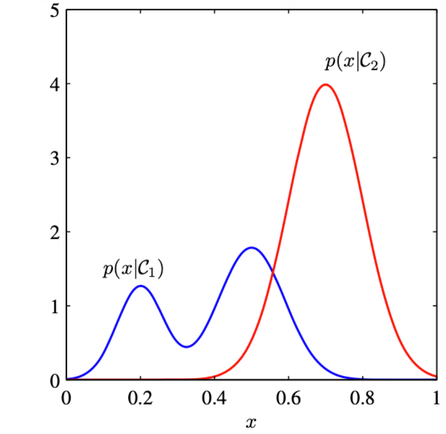
Tasks: (1) Find $p_\theta(C_1 \mid \mathbf{x})$, (2) Find $\theta = \{\mu_1, \mu_2, \Sigma, \pi_1\}$ using maximum likelihood,
(3) Generalisation to multiple classes, and (4) Different covariances for different classes?

Check: Are logistic classification and linear discriminant analysis the same thing?

Generative vs discriminative: comparison

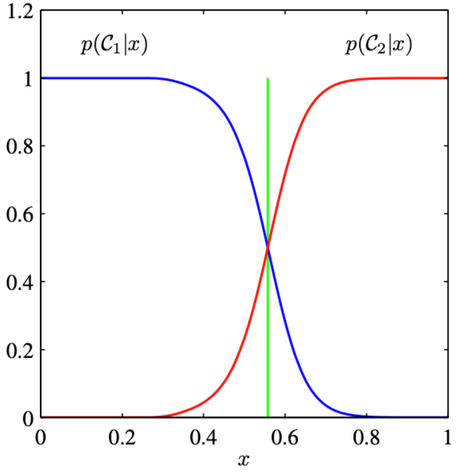
Generative

$$p_\theta(\mathbf{x}, y) = p_\theta(\mathbf{x} \mid y) p_\theta(y)$$



Discriminative

$$p_\theta(y \mid \mathbf{x})$$

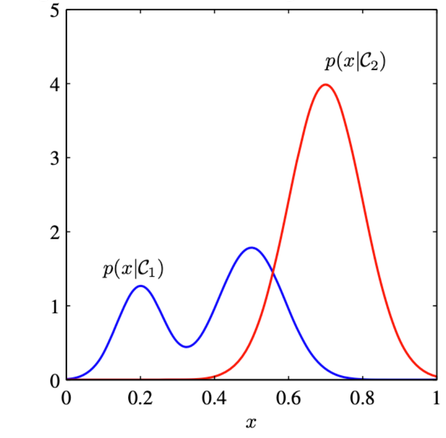


Murphy, Probabilistic ML: An Introduction

Generative vs discriminative: comparison

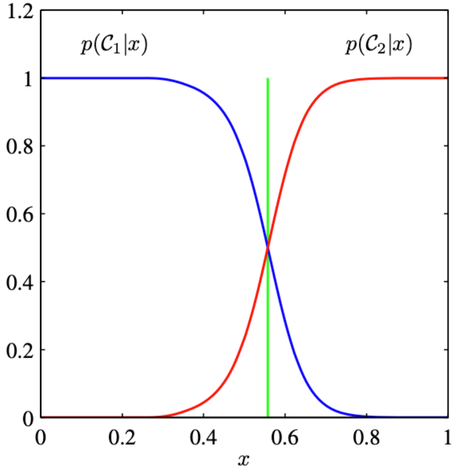
Generative

$$p_\theta(\mathbf{x}, y) = p_\theta(\mathbf{x} \mid y) p_\theta(y)$$



Discriminative

$$p_\theta(y \mid \mathbf{x})$$



9.4.1 Advantages of discriminative classifiers

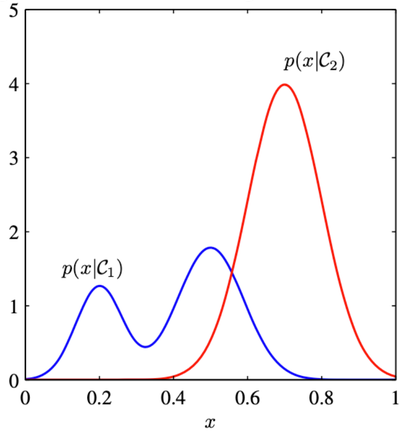
The main advantages of discriminative classifiers are as follows:

- **Better predictive accuracy**. Discriminative classifiers are often much more accurate than generative classifiers [NJ02]. The reason is that the conditional distribution $p(y|\boldsymbol{x})$ is often much simpler (and therefore easier to learn) than the joint distribution $p(y, \boldsymbol{x})$, as illustrated in Figure 9.8. In particular, discriminative models do not need to "waste effort" modeling the distribution of the input features.
- **Can handle feature preprocessing**. A big advantage of discriminative methods is that they allow us to preprocess the input in arbitrary ways. For example, we can perform a polynomial expansion of the input features, and we can replace a string of words with embedding vectors (see Section 20.5). It is often hard to define a generative model on such pre-processed data, since the new features can be correlated in complex ways which are hard to model.
- **Well-calibrated probabilities**. Some generative classifiers, such as naive Bayes (described in Section 9.3), make strong independence assumptions which are often not valid. This can result in very extreme posterior class probabilities (very near 0 or 1). Discriminative models, such as logistic regression, are often better calibrated in terms of their probability estimates, although they also sometimes need adjustment (see e.g., [NMC05]).

Generative vs discriminative: comparison

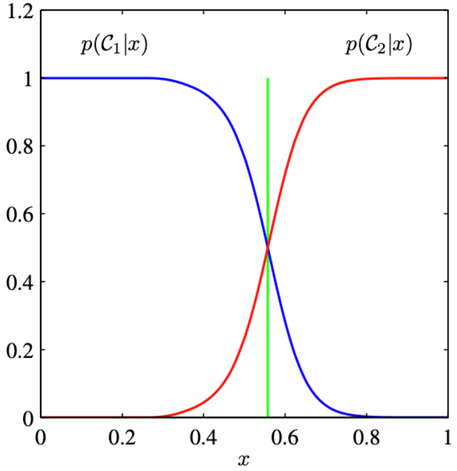
Generative

$$p_\theta(\mathbf{x}, y) = p_\theta(\mathbf{x} \mid y) p_\theta(y)$$



Discriminative

$$p_\theta(y \mid \mathbf{x})$$



9.4.2 Advantages of generative classifiers

The main advantages of generative classifiers are as follows:

- **Easy to fit.** Generative classifiers are often very easy to fit. For example, in Section 9.3.2, we show how to fit a naive Bayes classifier by simple counting and averaging. By contrast, logistic regression requires solving a convex optimization problem (see Section 10.2.3 for the details), and neural nets require solving a non-convex optimization problem, both of which are much slower.

- **Can easily handle missing input features.** Sometimes some of the inputs (components of $\boldsymbol{x}$) are not observed. In a generative classifier, there is a simple method for dealing with this, as we show in Section 1.5.5. However, in a discriminative classifier, there is no principled solution to this problem, since the model assumes that $\boldsymbol{x}$ is always available to be conditioned on.

- **Can fit classes separately.** In a generative classifier, we estimate the parameters of each class conditional density independently (as we show in Section 9.3.2), so we do not have to retrain the model when we add more classes. In contrast, in discriminative models, all the parameters interact, so the whole model must be retrained if we add a new class.

- **Can handle unlabeled training data.** It is easy to use generative models for semi-supervised learning, in which we combine labeled data $\mathcal{D}_{xy} = \{(\boldsymbol{x}_n, y_n)\}$ and unlabeled data, $\mathcal{D}_x = \{\boldsymbol{x}_n\}$. However, this is harder to do with discriminative models, since there is no uniquely optimal way to exploit $\mathcal{D}_x$.

- **May be more robust to spurious features**. A discriminative model $p(y|\boldsymbol{x})$ may pick up on features of the input $\boldsymbol{x}$ that can discriminate different values of y in the training set, but which are not robust and do not generalize beyond the training set. These are called **spurious features** (see e.g., [Arj21; Zho+21]). By contrast, a generative model $p(\boldsymbol{x}|y)$ may be better able to capture the causal mechanisms of the underlying data generating process; such causal models can be more robust to distribution shift (see e.g., [Sch19; LBS19; LN81]).

Overview

1. Recap: Linear regression
2. Discriminative: From least squares to binary logistic classification
3. Discriminative: From binary to multi-class classification
4. Generative model: linear discriminant analysis
5. [Optional] Evaluation
6. [Optional] Linearly separable data - perceptron algorithm

Three approaches to classification:

Learning a discriminant function, directly mapping $\mathbf{x}$ to class label y

Building a discriminative model, learning $p_\theta(\mathbf{y} \mid \mathbf{x})$

Building a generative model,
learning $p_\theta(\mathbf{x} \mid \mathbf{y})$ and $p_\phi(\mathbf{y})$ then find $p_{\theta,\phi}(\mathbf{y} \mid \mathbf{x})$ using Bayes' rule.

Binary classification - confusion matrix

True label

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

Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - confusion matrix

True label

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

Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - confusion matrix

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

Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - confusion matrix

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

Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - confusion matrix

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

Assuming the labels are -1 and 1, instead of 0 and 1

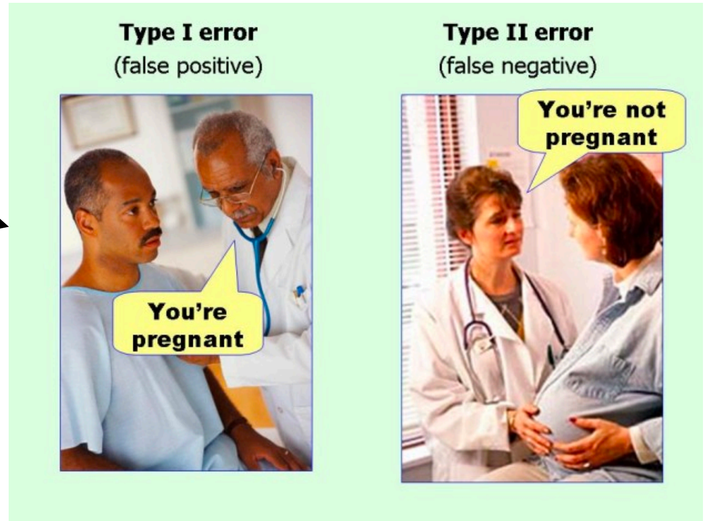
Binary classification - confusion matrix

		True label		
		$y = -1$	$y = 1$	Total
Predicted label	$\hat{y} = -1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
	$\hat{y} = 1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
	Total	N_n	N_p	N

Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - confusion matrix

		True label $y=-1$	True label $y=1$	Total
Predicted label	$\hat{y}=-1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
	$\hat{y}=1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
	Total	N_n	N_p	N



Assuming the labels are -1 and 1, instead of 0 and 1

Binary classification - popular metrics

Predicted label \ True label	$y = -1$	$y = 1$	Total
$\hat{y} = -1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
$\hat{y} = 1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
Total	N_n	N_p	N

Binary classification - popular metrics

		True label		
		$y = -1$	$y = 1$	Total
Predicted label	$\hat{y} = -1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
	$\hat{y} = 1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
	Total	N_n	N_p	N

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{N}$$

$$\text{Error} = \frac{\text{FP} + \text{FN}}{N}$$

Binary classification - popular metrics

		True label: $y = -1$	True label: $y = 1$	Total
Predicted label	$\hat{y} = -1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
	$\hat{y} = 1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
	Total	N_n	N_p	N

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{N} \qquad \text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

$$\text{Error} = \frac{\text{FP} + \text{FN}}{N} \qquad \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

Binary classification - popular metrics

		True label		
		$y = -1$	$y = 1$	Total
Predicted label	$\hat{y} = -1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
	$\hat{y} = 1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
	Total	N_n	N_p	N

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

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

Binary classification - popular metrics

	True label $y=-1$	$y=1$	Total
Predicted label $\hat{y}=-1$	True negative (TN)	False negative (FN)	$\hat{N}_n$
$\hat{y}=1$	False positive (FP)	True positive (TP)	$\hat{N}_p$
Total	N_n	N_p	N

Questions: compute these metrics for

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

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

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

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
FN/N*	False omission rate
P/*n*	Prevalence
(FN + FP)/*n*	*Misclassification rate*
(TN + TP)/*n*	Accuracy, 1 − misclassification rate
2TP/(P* + P)	F_1 *score*
$(1 + \beta^2)$TP/$((1 + \beta^2)$TP + β^2FN + FP)	F_β *score*

In this table: N is Nn, P is Np, n is N

Binary classification - too many metrics?

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We could have a whole course on metrics!

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Binary classification - too many metrics?

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Need to consider down-stream applications, e.g. in medical domain, FNs are costly but FPs result in unnecessary further tests.

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Binary classification - too many metrics?

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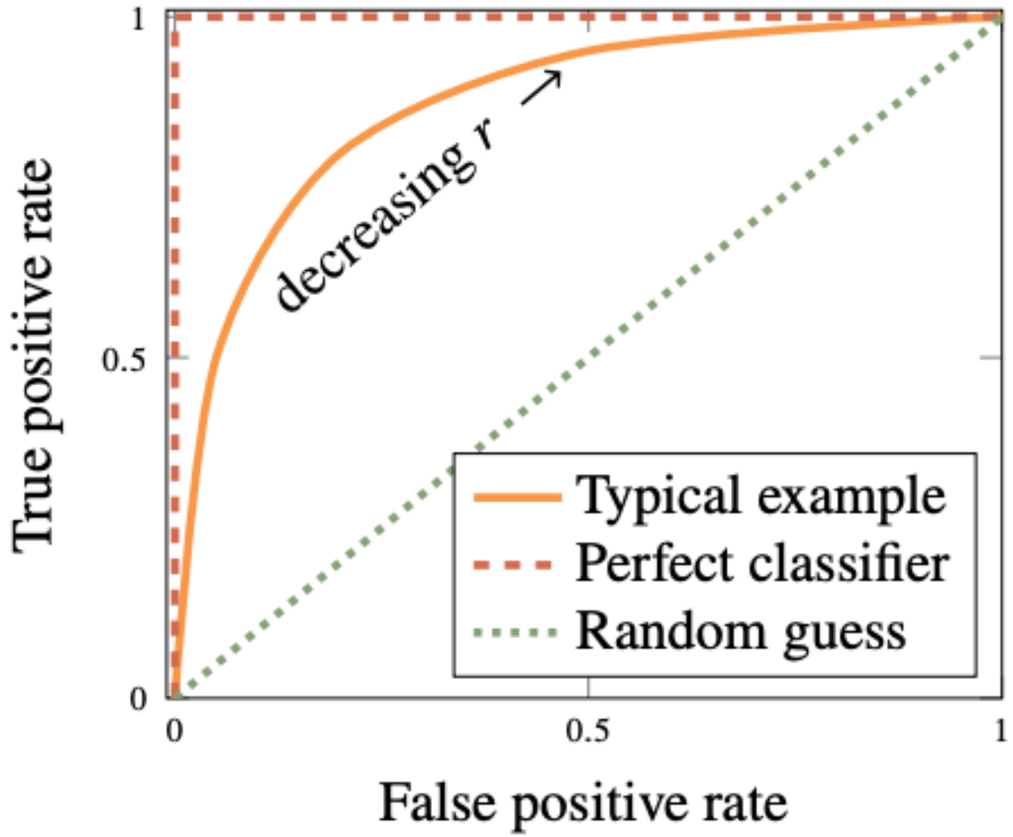
Need to consider down-stream applications, e.g. in medical domain, FNs are costly but FPs result in unnecessary further tests.

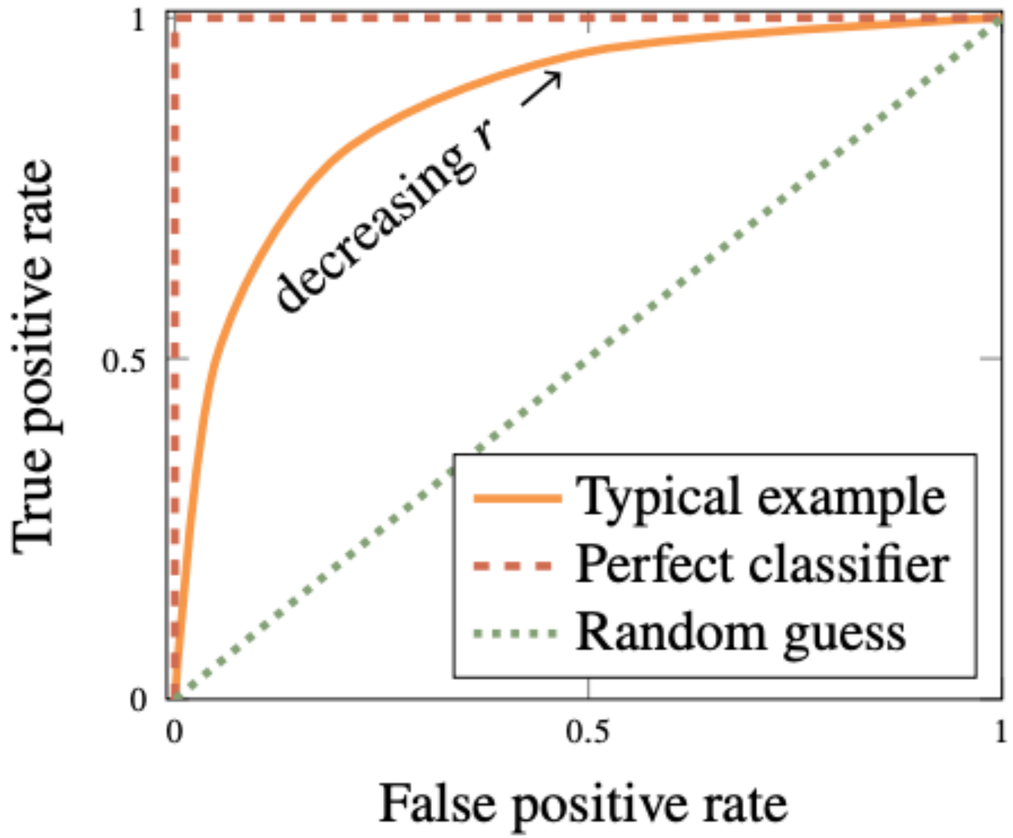
Accuracy and error are not useful for imbalanced classes

In this table: N is Nn, P is Np, n is N

Binary classification - Receiver Operating Characteristic



Binary classification - Receiver Operating Characteristic



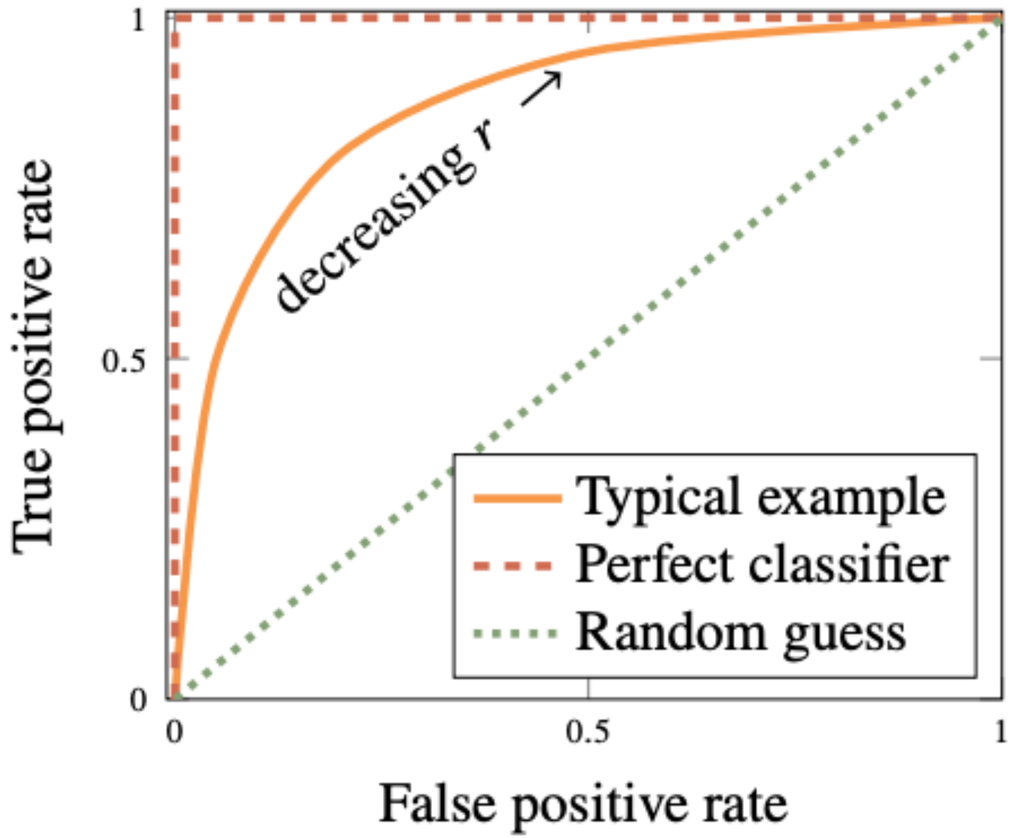
Consider a binary classification example, at test time:

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

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

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

Binary classification - Receiver Operating Characteristic



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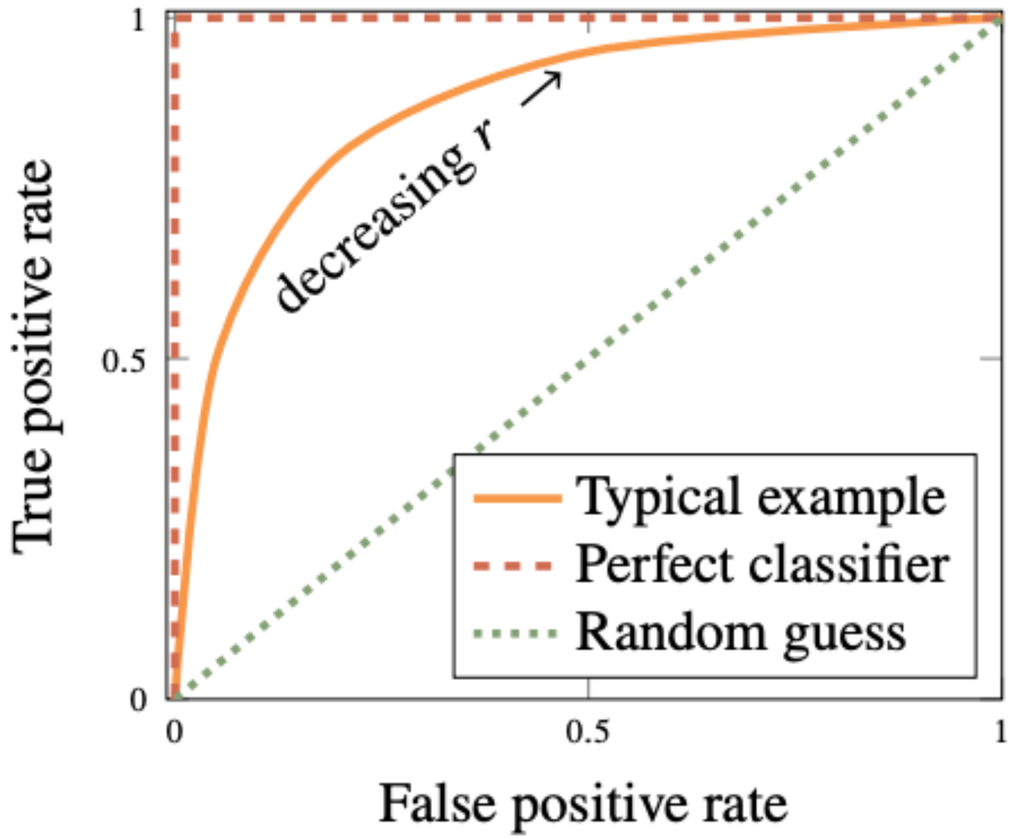
For each threshold between 0.0 and 1.0, we make decisions for all test points, construct the confusion matrix, calculate TPR and FPR, and draw a corresponding point on the **ROC** chart.

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

Binary classification - Receiver Operating Characteristic



ROC curve is used to select an *operating point*, aka the threshold of the classifier.

We can compare multiple classifiers using their ROC curves. Better classifiers tend to have higher Area Under the Curve (AUC).

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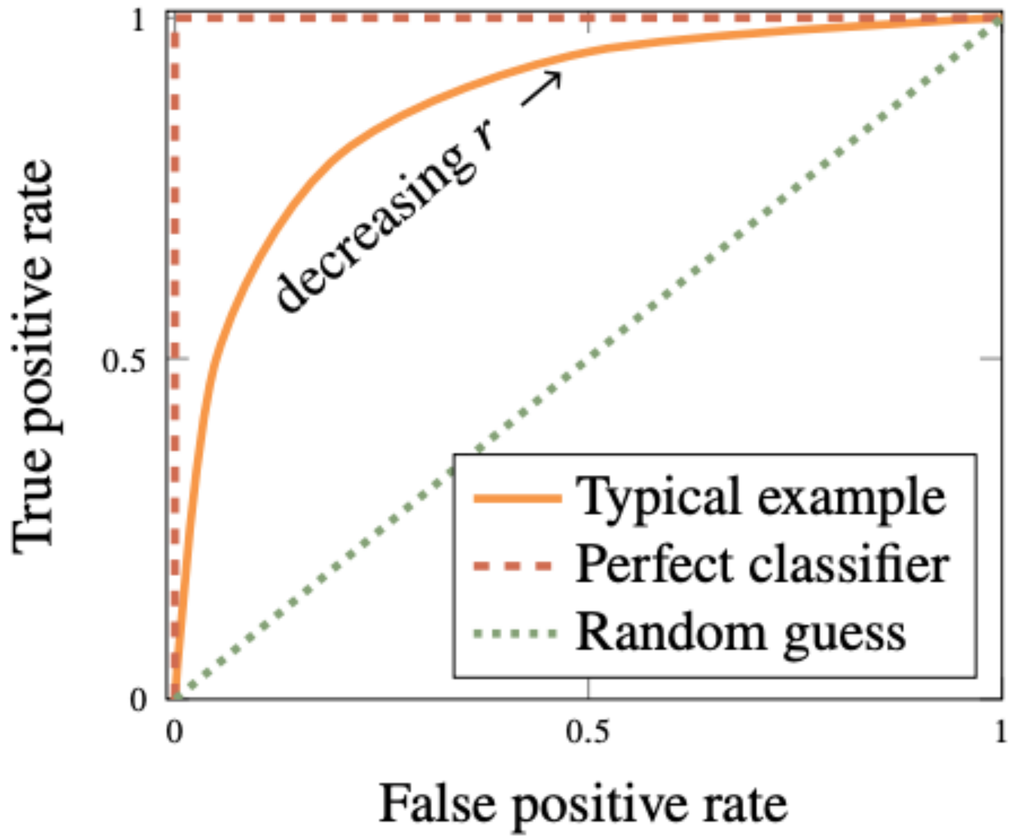
Binary classification - Receiver Operating Characteristic



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

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

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.

Model - *step* `squashing` function and criterion

Model - *step* `squashing` function and criterion

Linear mapping:

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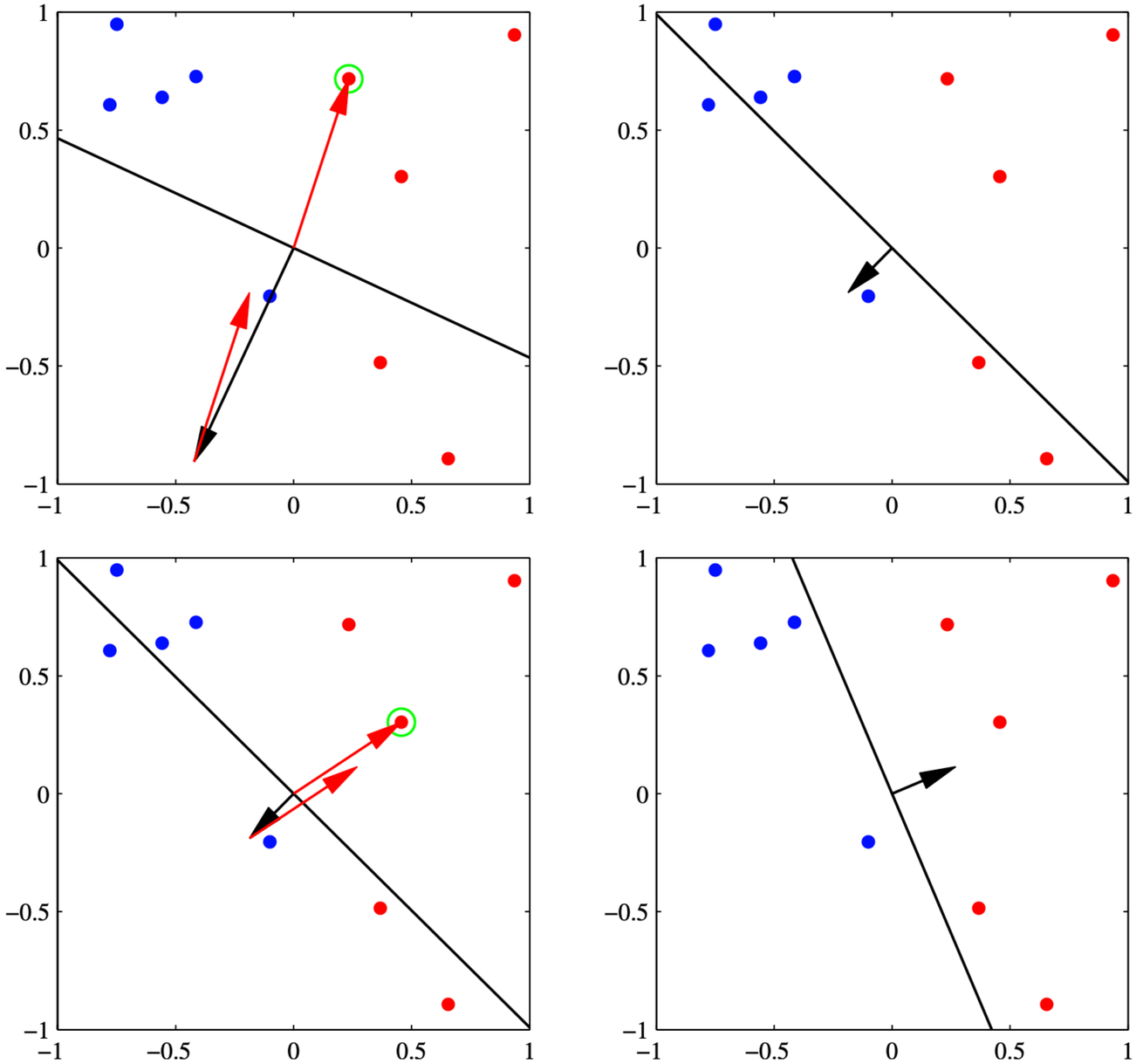
SGD update: *for each misclassified example,* $\theta^{t+1} = \theta^t + x_n y_n$. Derive this!

Perceptron algorithm - an example



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