Lecture 5: Supervised Learning Methods

Introduction to Artificial Intelligence and Machine Learning (IntroAIML)

Michael Mommert, University of St. Gallen

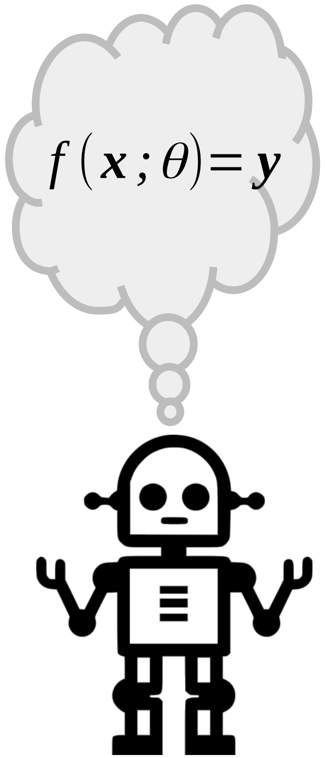
Today's lecture

Linear models

Nearest Neighbor models

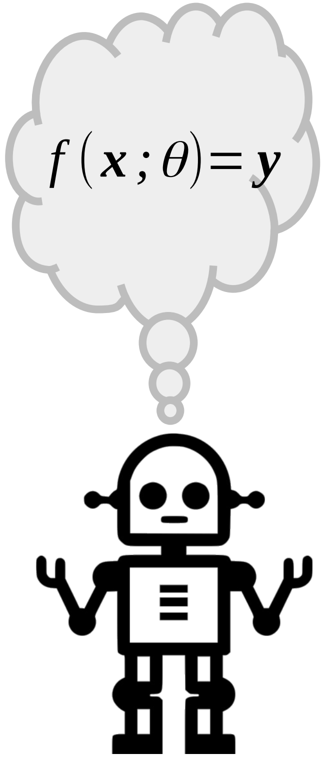
Tree-based models

Reminder: general supervised learning pipeline



Reminder: general supervised learning pipeline

1) Feature engineering: raw data → features



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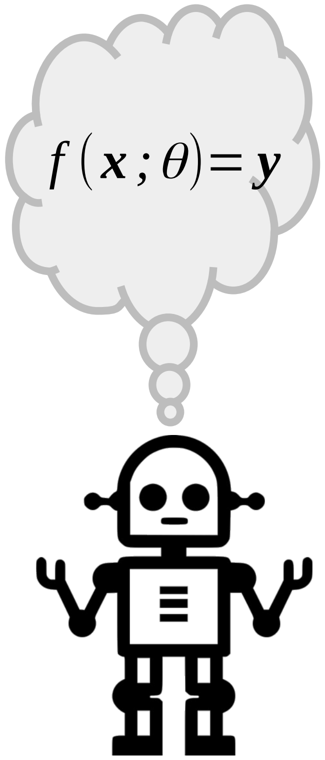

Reminder: general supervised learning pipeline

1) Feature engineering: raw data → features

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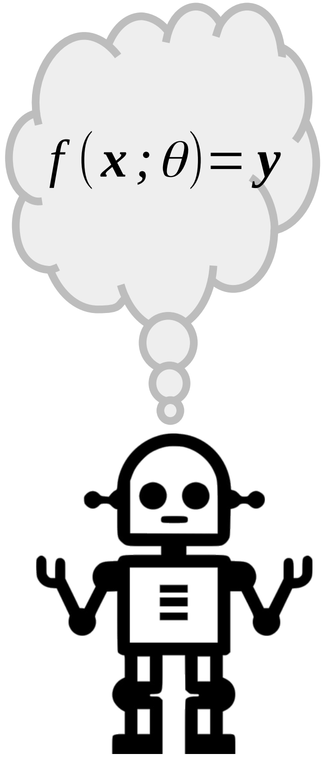
3) Data splitting → training, validation, test data



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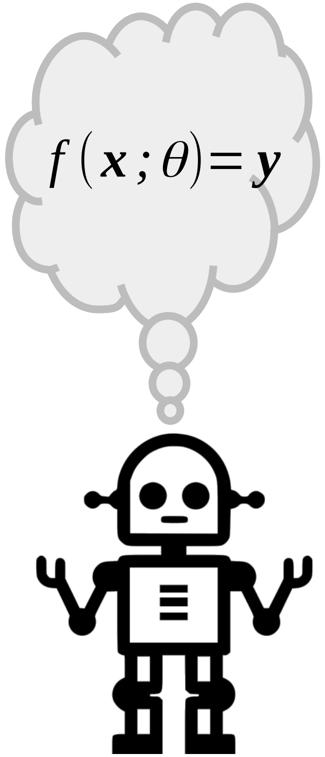

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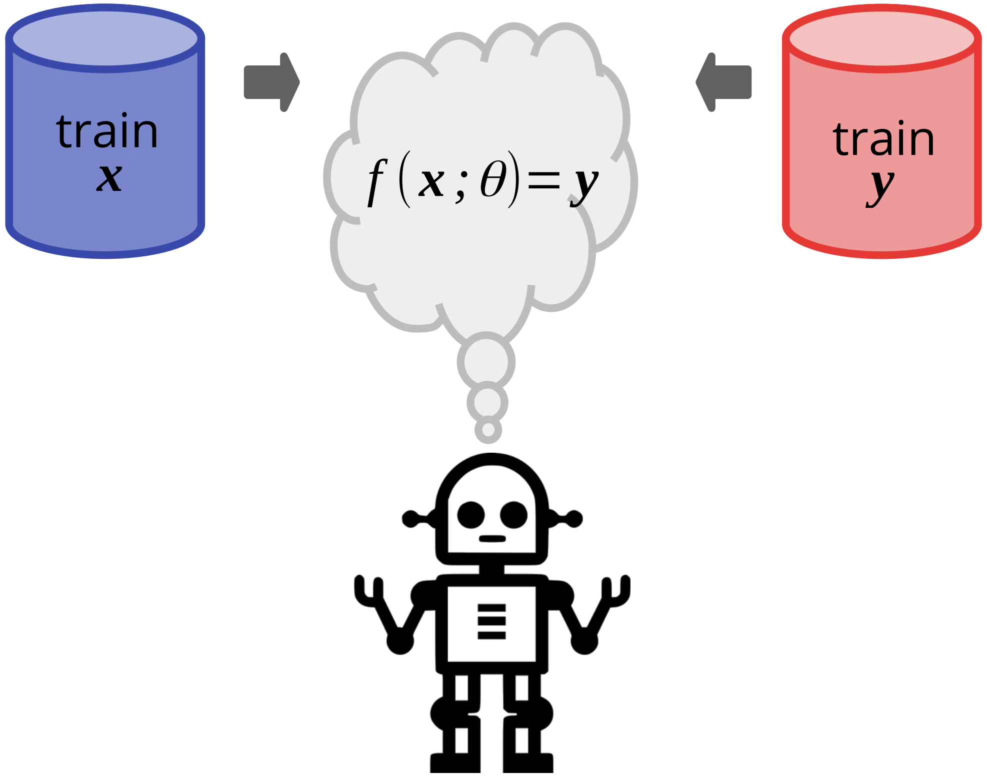

model training

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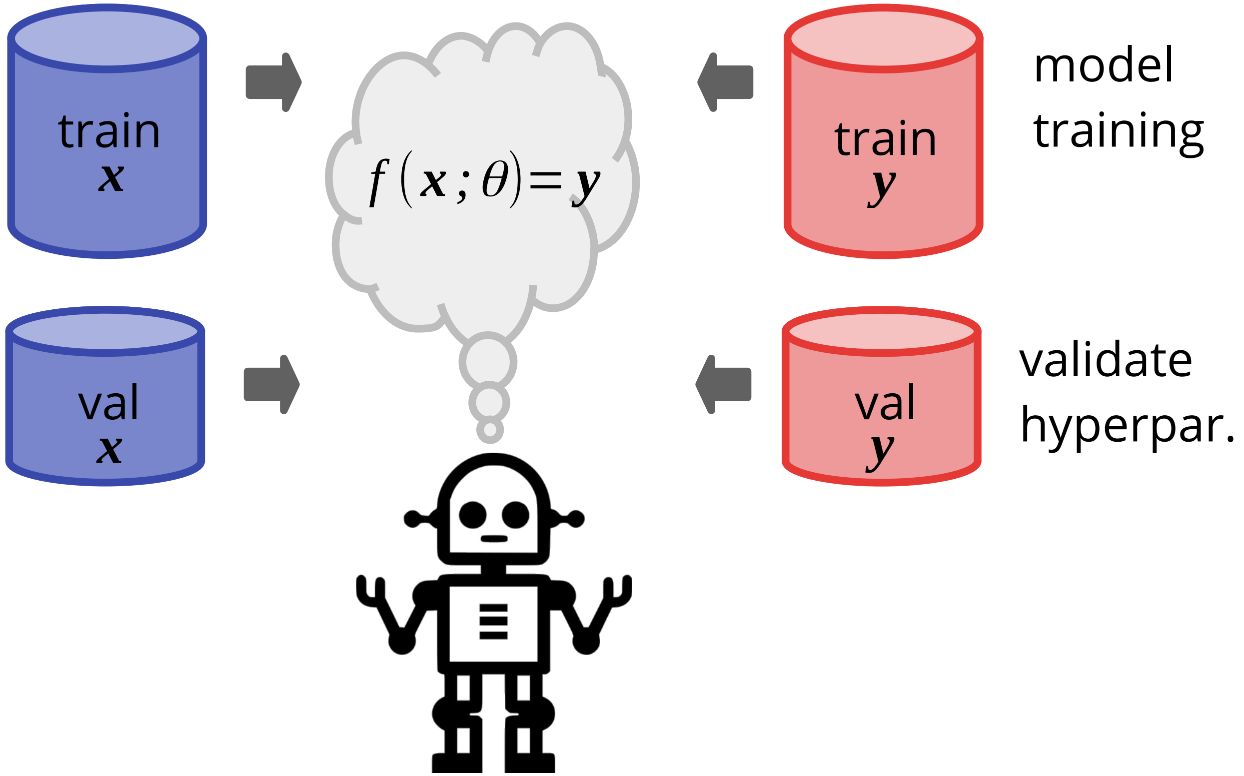
6) Evaluate model on validation data



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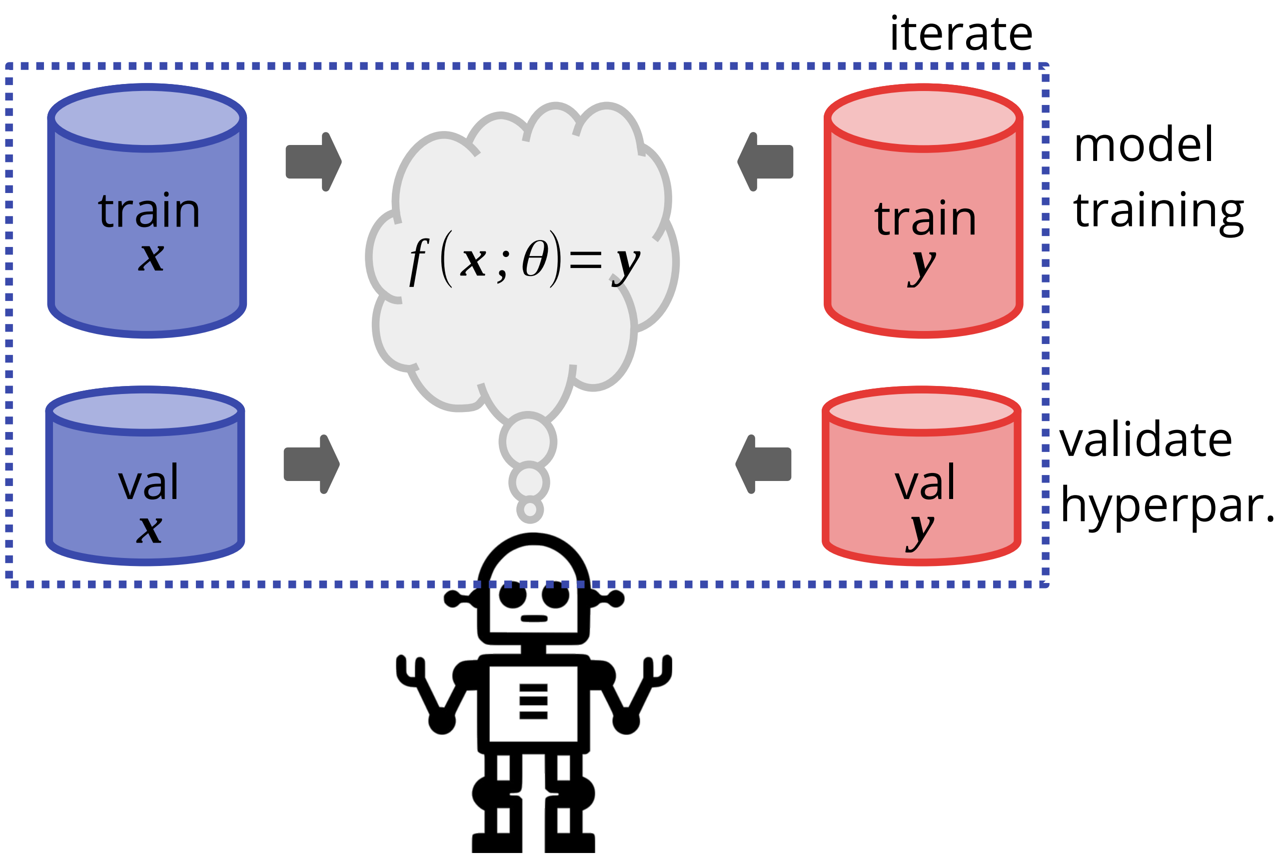

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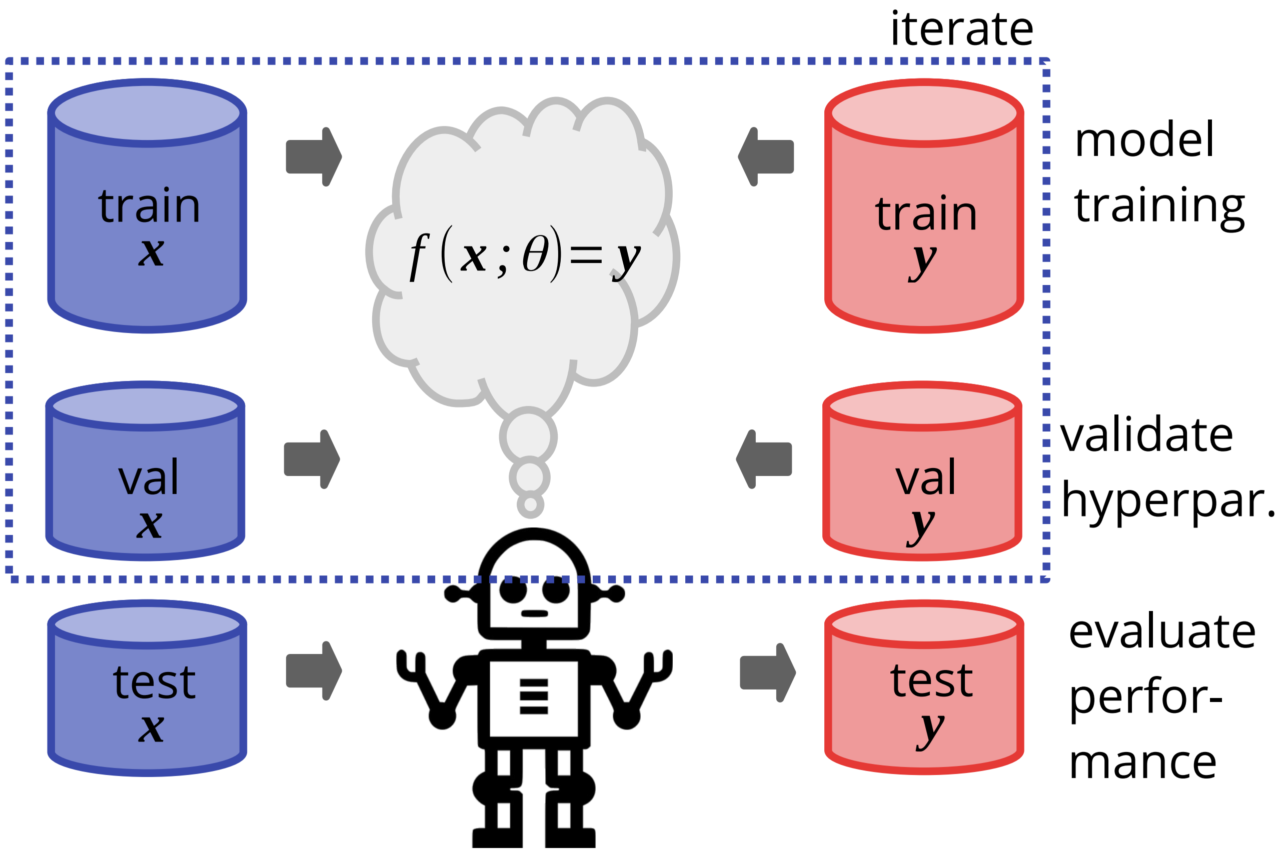
→ report test data performance



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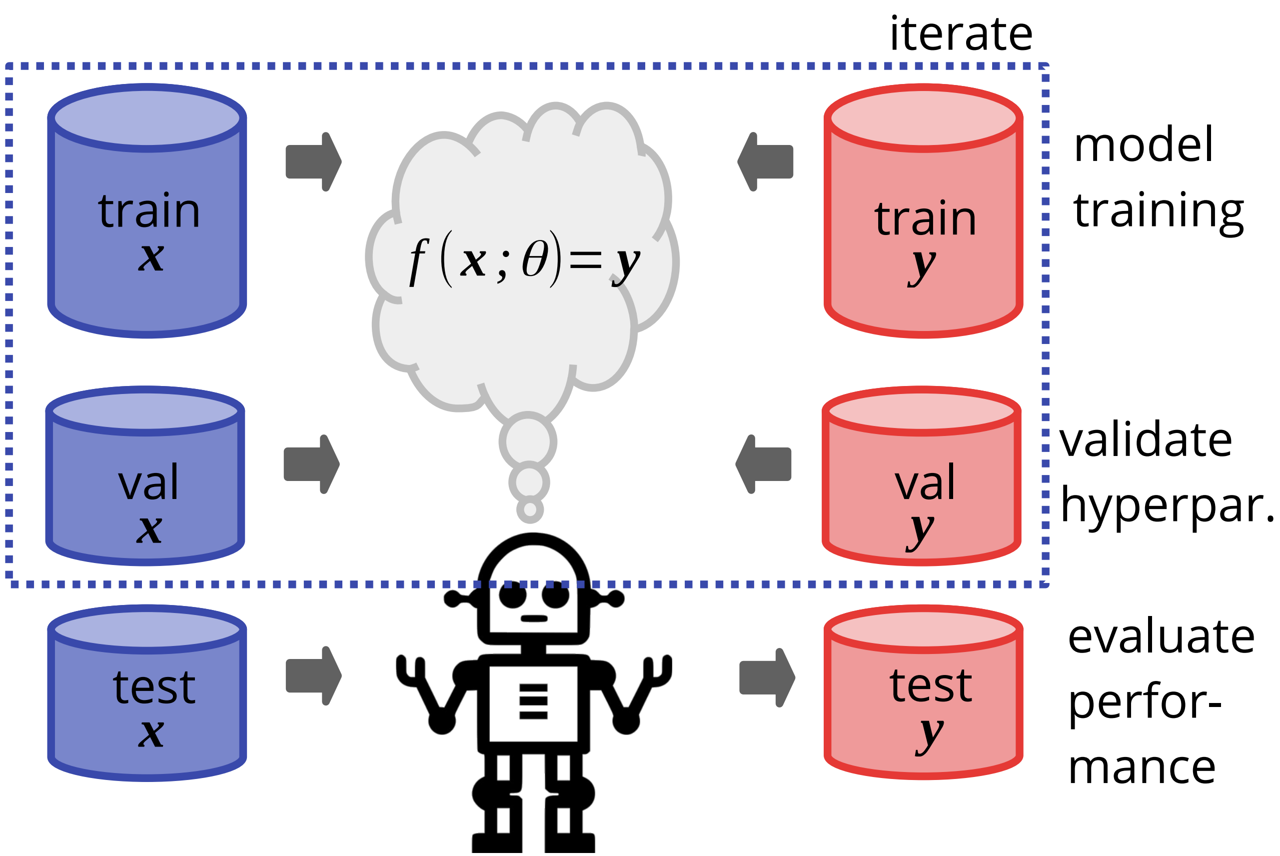
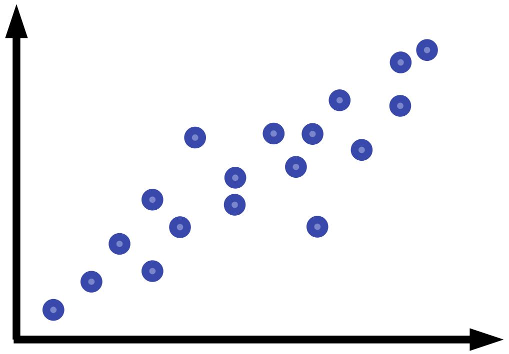
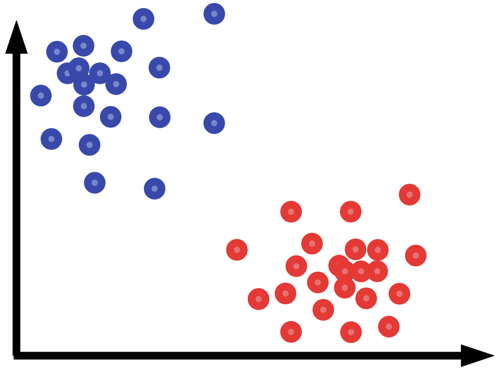


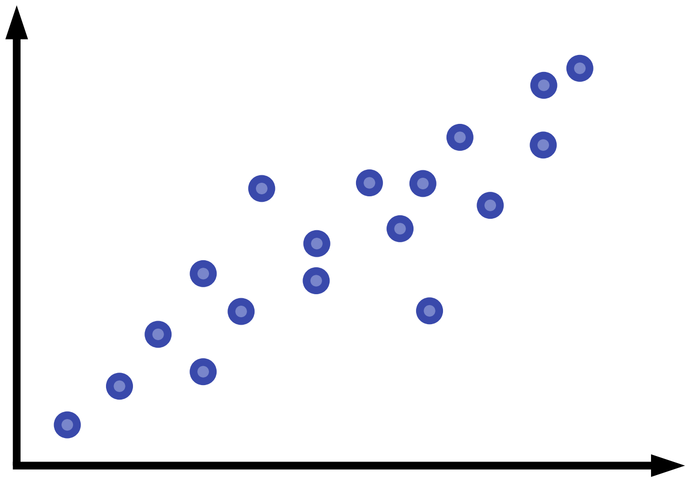
Goal: maximize performance while preventing overfitting!

Linear models

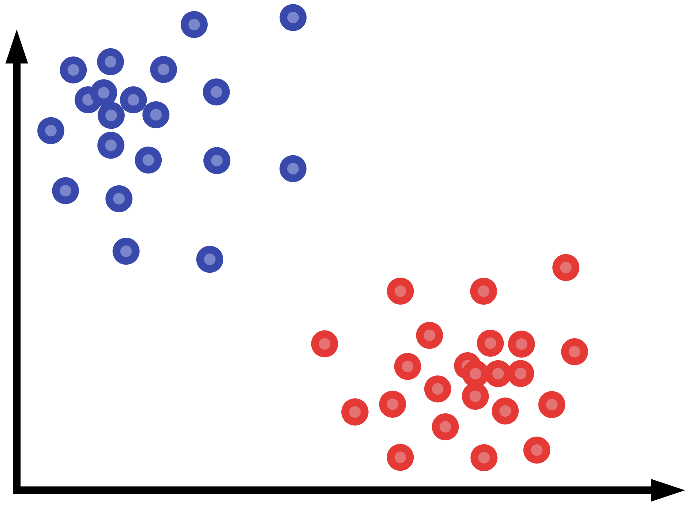




Linear models assume **linearity** in the underlying data. They are rather simple but convey many of the concepts utilized in other, more complex models.



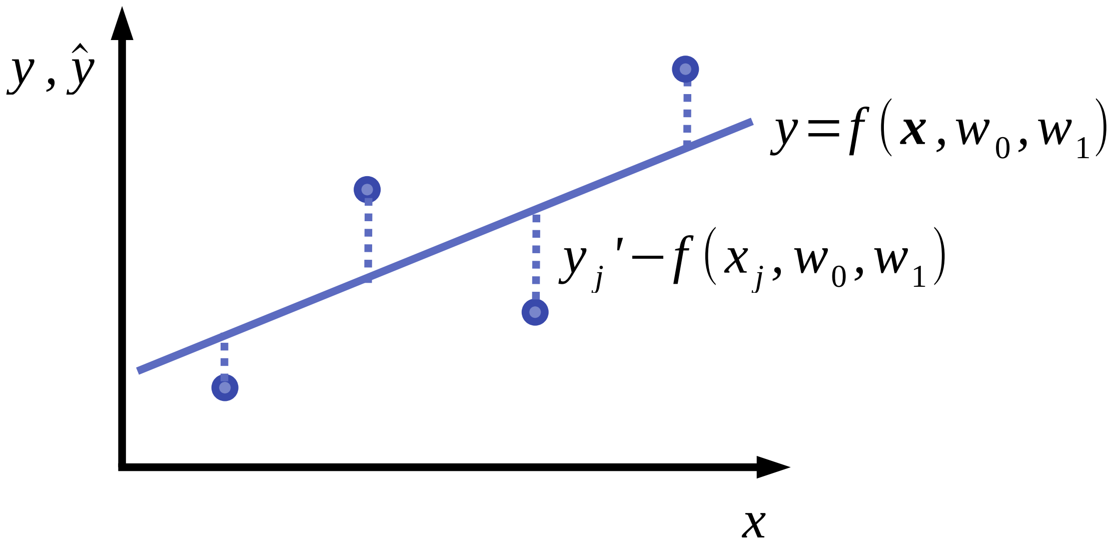
Linear regression



Linear classification

Linear regression (univariate)

Find weights w_0 and w_1 so that the linear function $f(x)=w_1 x+w_o$ with input x and output y best fits the data containing ground-truth values y'.



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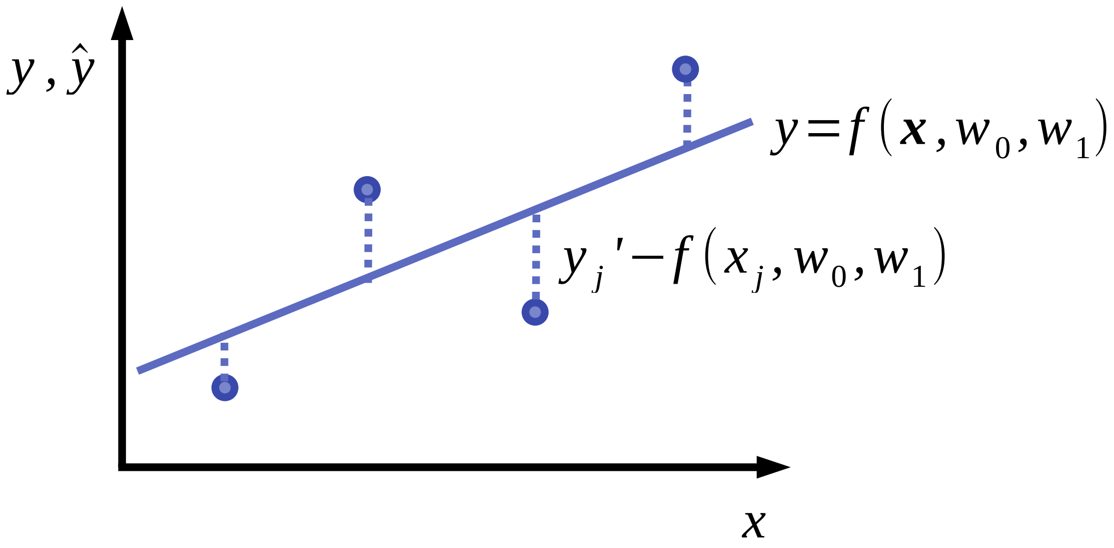
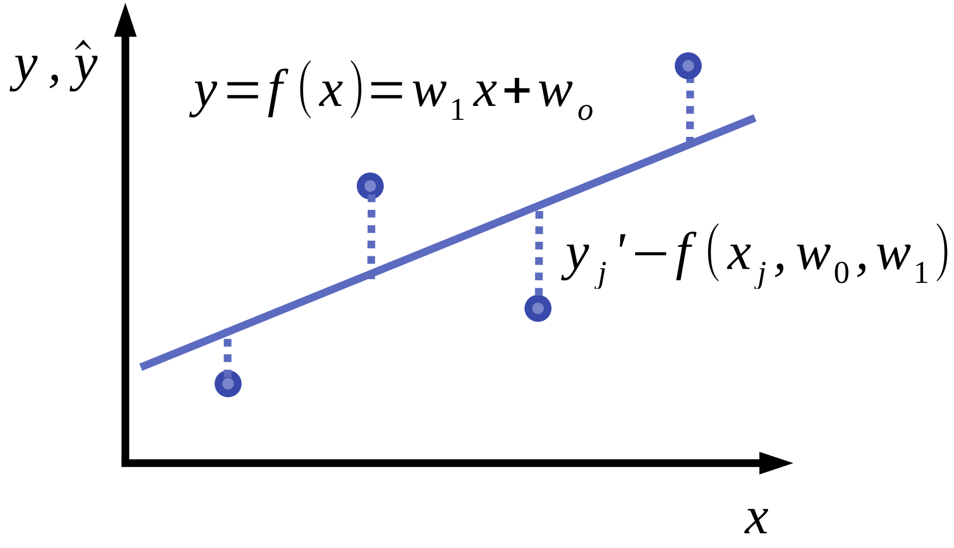


How can we learn w_0 and w_1 from data?

Linear regression (univariate) – Least squares fitting

Idea: minimize squared errors of prediction with respect to ground truth for each data point:

for data point j: $[y_j' - f(x_j, w_0, w_1)]^2$



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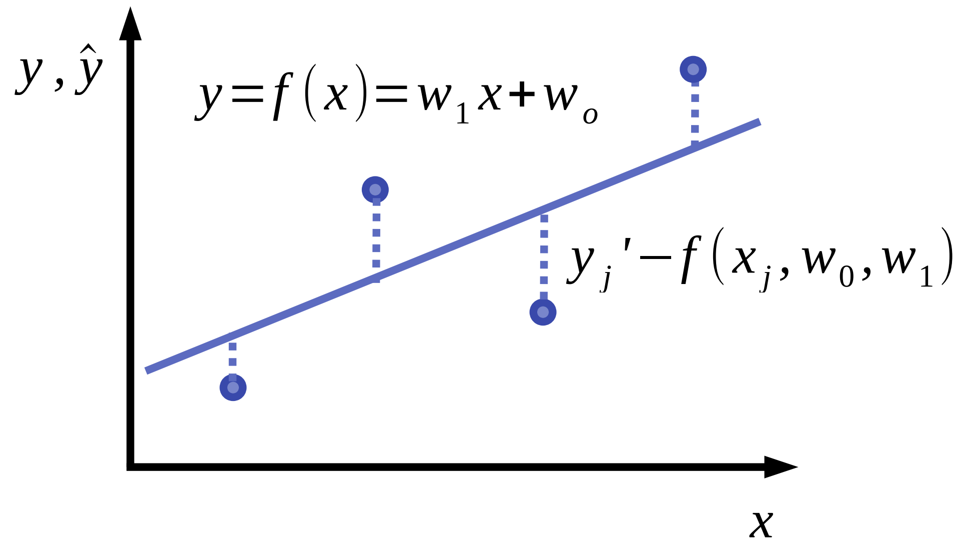

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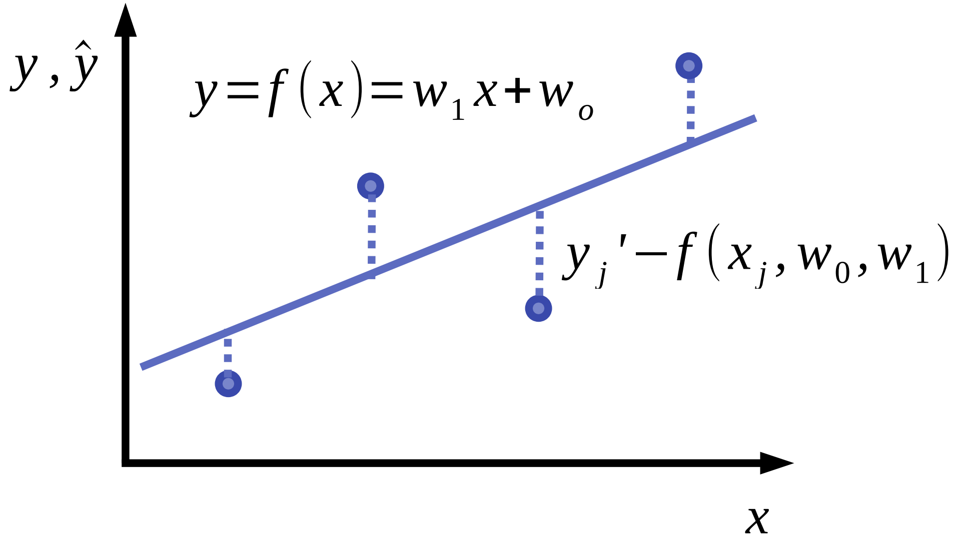

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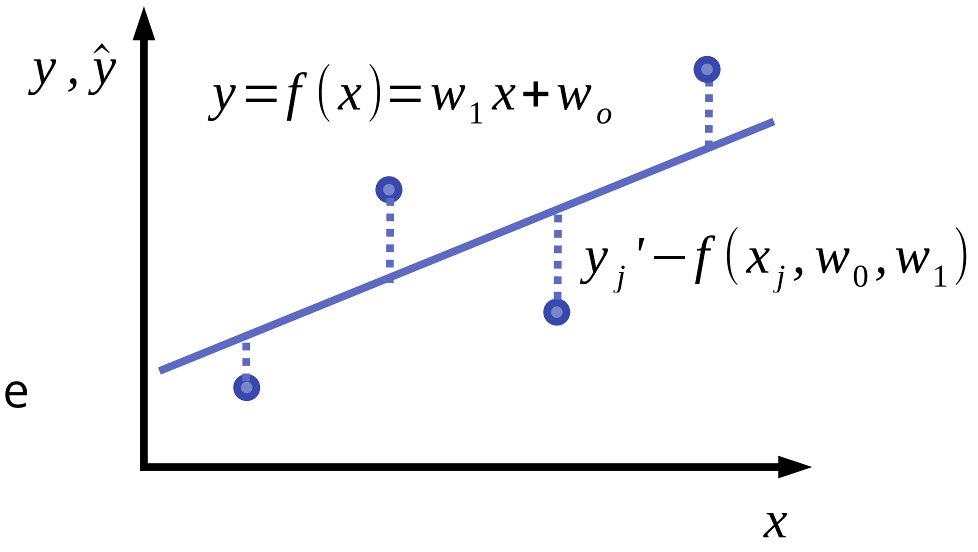

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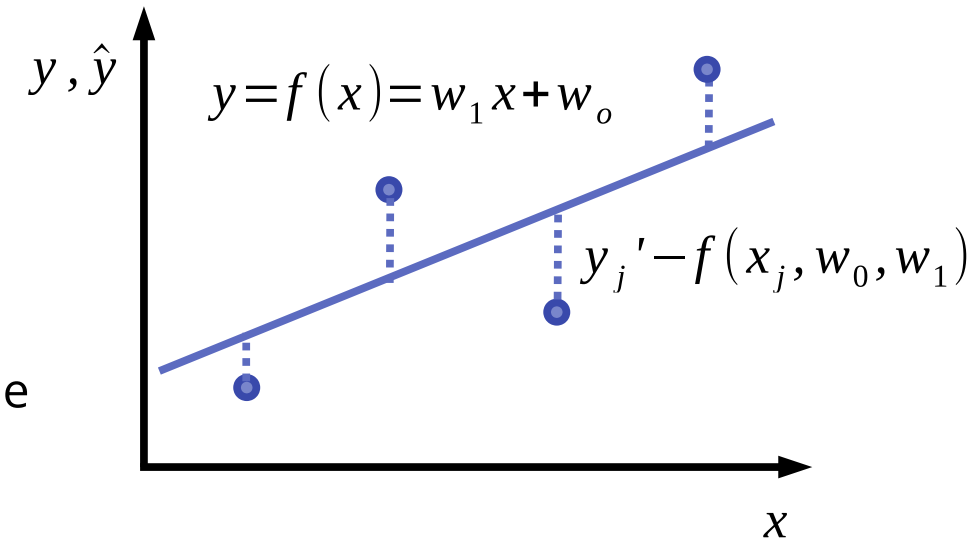

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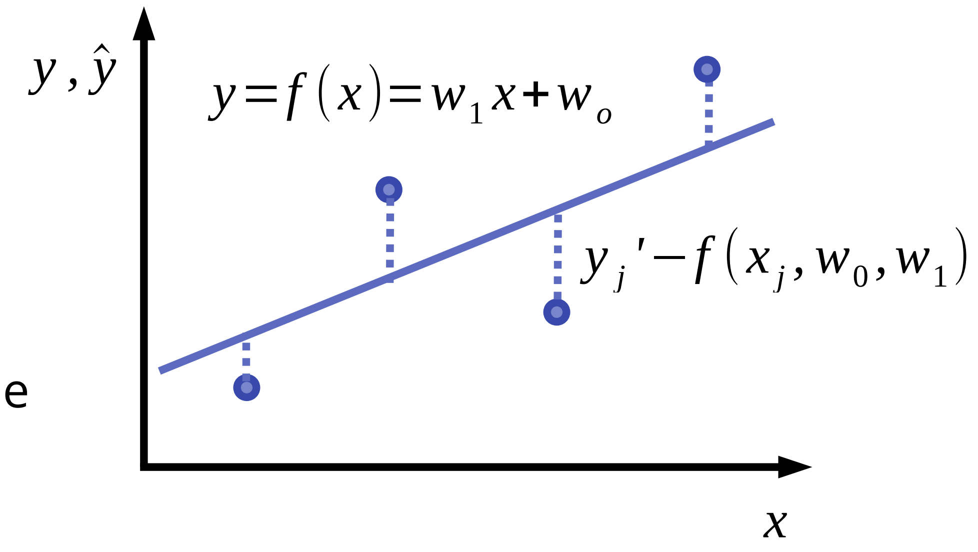

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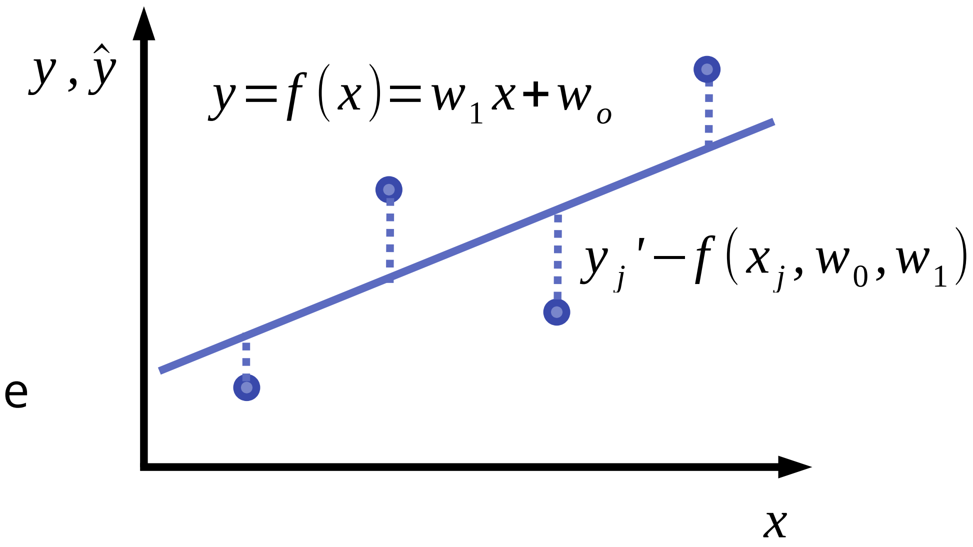

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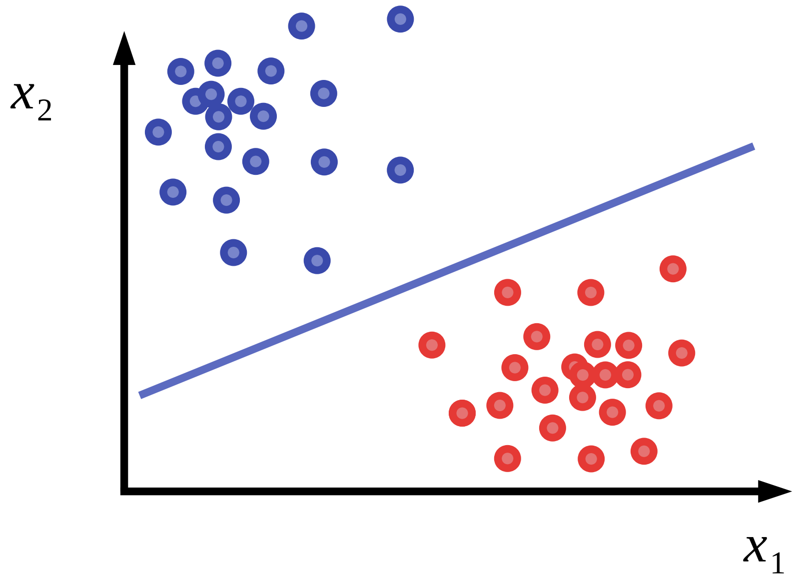
Least-squares + linear model function: the resulting minimum of the Loss function is **global**, i.e., the "learns" immediately the best-possible solution!

Linear classifier (two-dimensional case)

Linear functions can also be used as a classifier if the data are linearly separable.



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Define decision boundary $f(\boldsymbol{x},\boldsymbol{w}) = \boldsymbol{w}\,\boldsymbol{x} = w_0 + w_1 x_1 + w_2 x_2$
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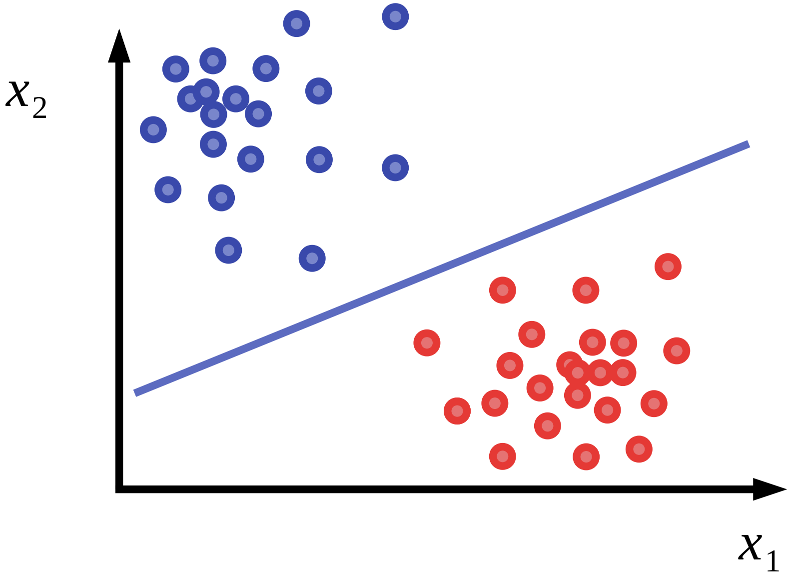

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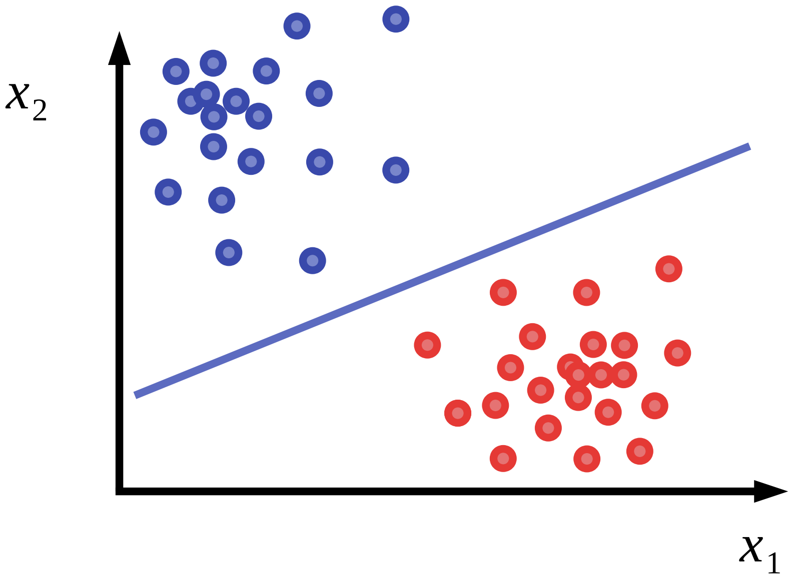
Class 1: $f(\boldsymbol{x}, \boldsymbol{w}) \geq 0$



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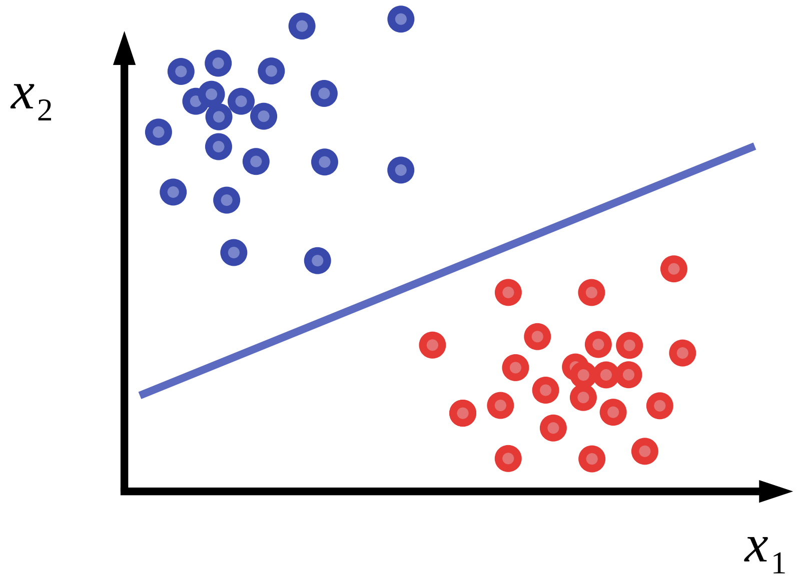

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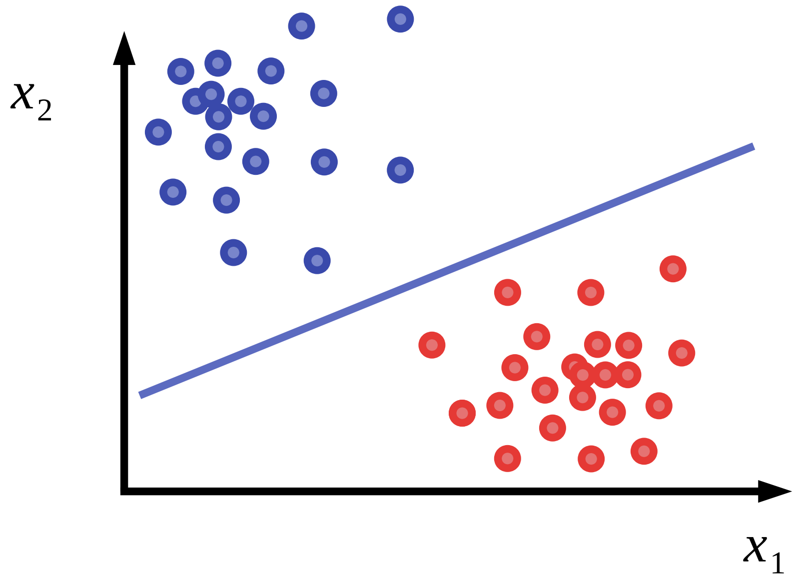
We can define class assignments through a threshold function:

$$\bar{f}(\boldsymbol{x},\boldsymbol{w})=\begin{cases} 1 \text{ if } f(\boldsymbol{x},\boldsymbol{w})\geq 0 \\ 0 \text{ if } f(\boldsymbol{x},\boldsymbol{w})<0 \end{cases}$$



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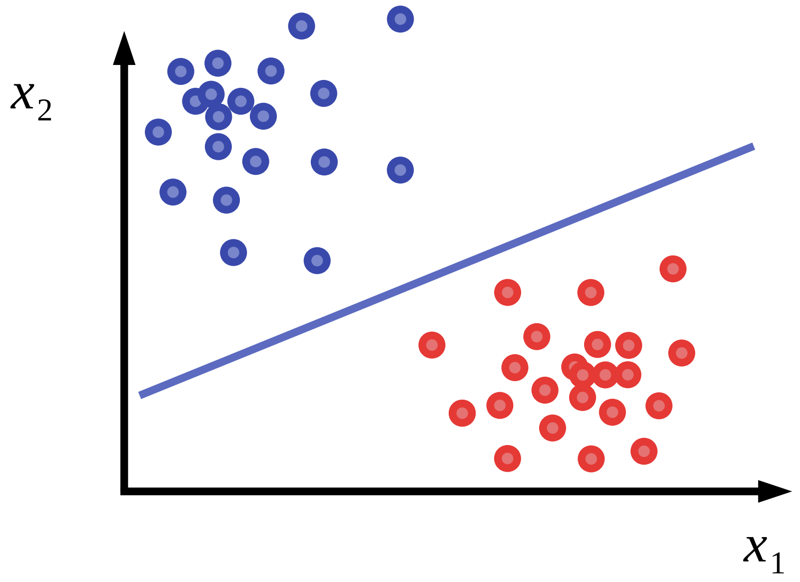
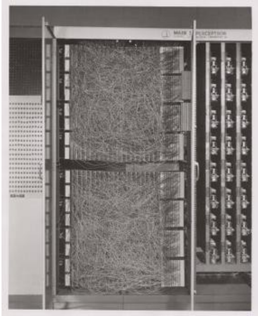


How can we learn $\boldsymbol{w}$ from data?

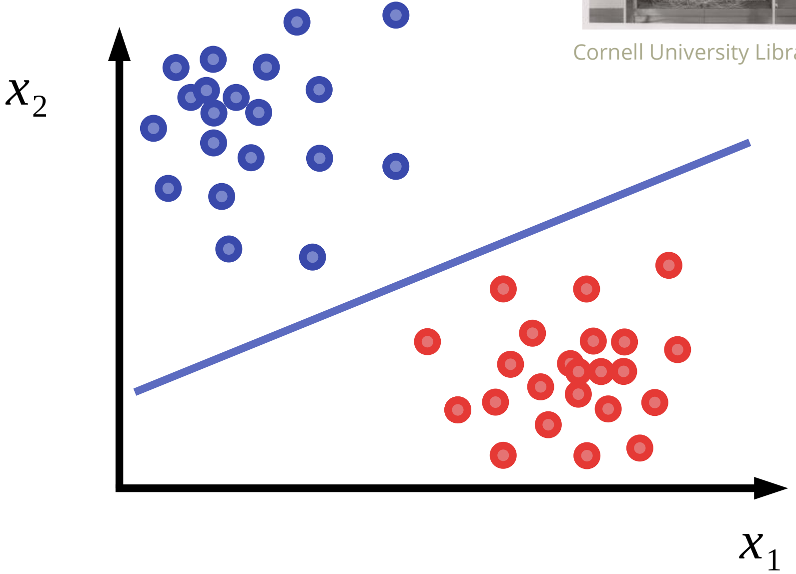
Linear classifier (two-dimensional case) – Perceptron learning rule



We define the following algorithm as the **Perceptron learning rule**:

We consider each data point, consisting of $\boldsymbol{x}$ and ground-truth label y' and check whether the prediction from $\bar{f}(\boldsymbol{x},\boldsymbol{w})$ is correct, or not. If…

- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=y$, then do nothing.
- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=0$ but $y'=1$, then increase w_i if $x_i \geq 0$, or vice versa.
- $\bar{f}(\boldsymbol{x},\boldsymbol{w})=1$ but $y'=0$, then decrease w_i if $x_i \geq 0$, or vice versa.



Weights are adjusted by a step size that is called the **learning rate**. By iteratively running this algorithm over your training data multiple times, the weights can be learned so that the model performs properly. A solution is “learned” iteratively here.

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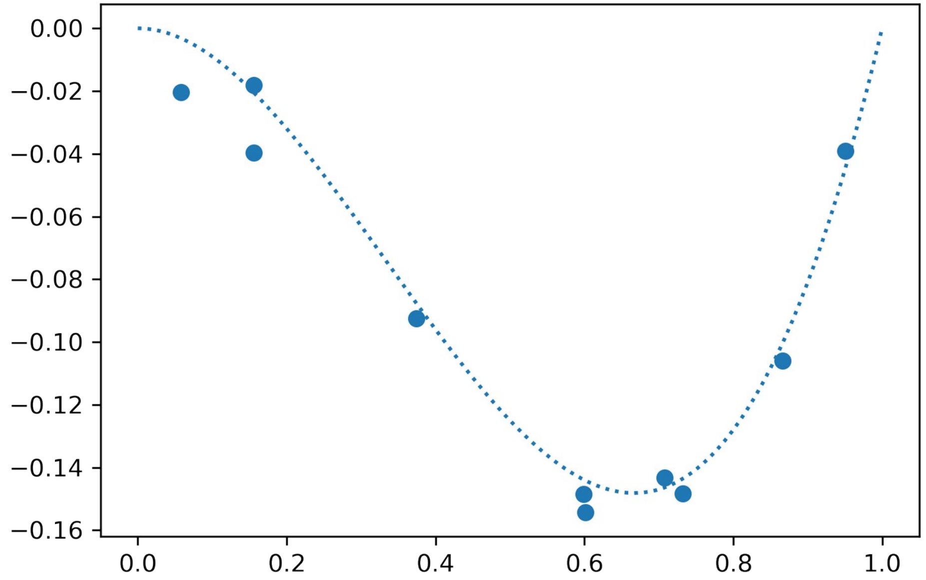
For more capacity, we can change the base function to a polynomial: $f(x) = w_0 + w_1 x + w_2 x^2 + \ldots = \sum_{i=0}^{p} w_i x^i$



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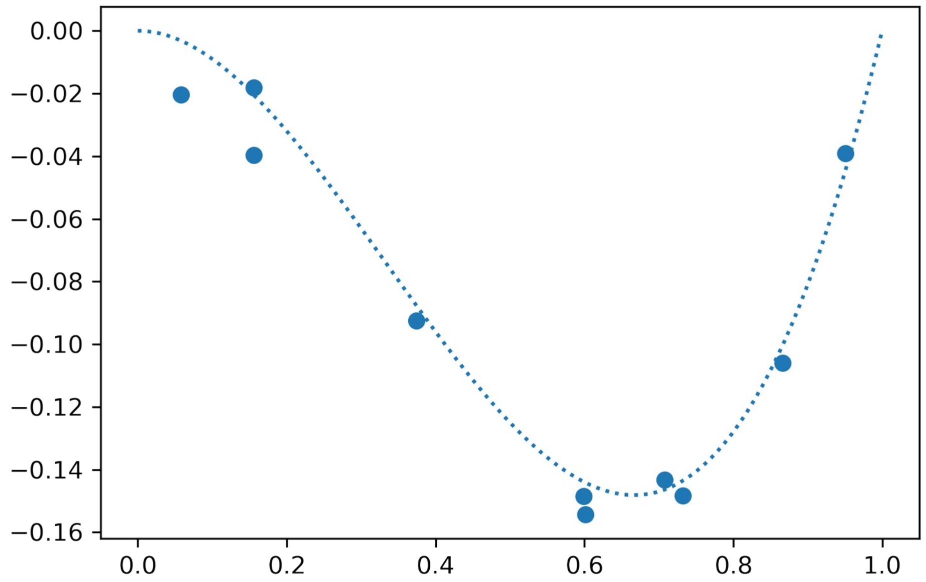

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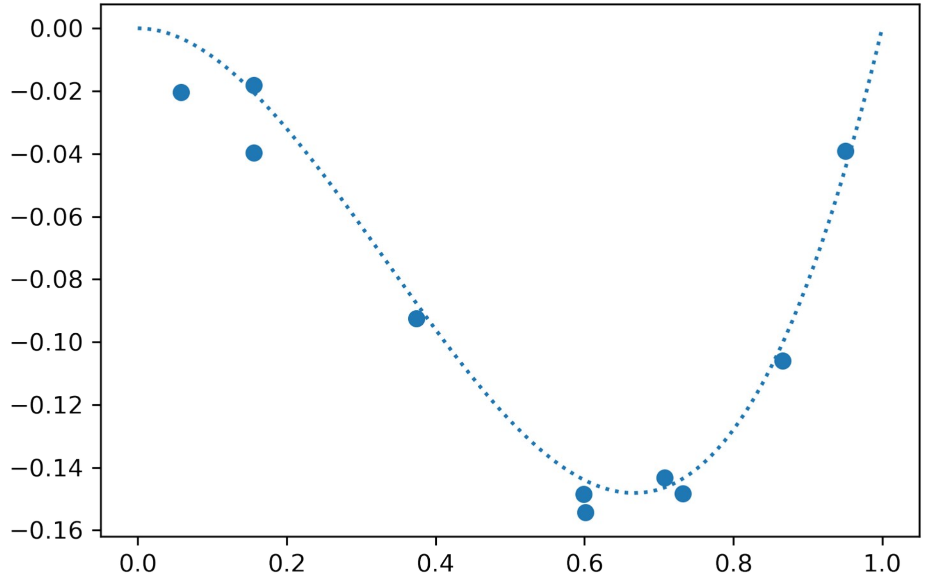
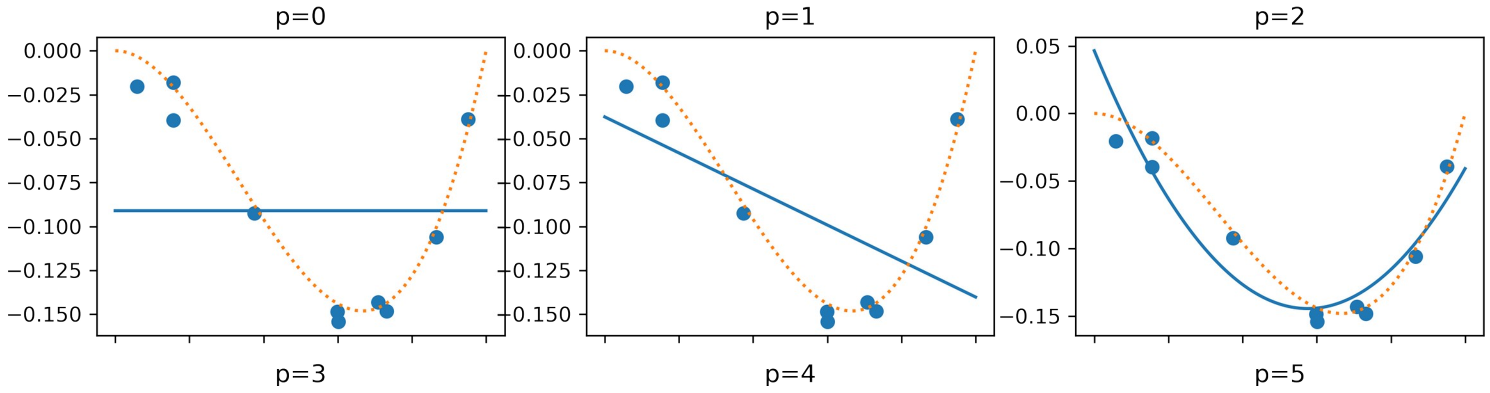
We can compute the parameters w_i to minimize the loss with a closed-form expression. This is by default the best possible solution.



Polynomial regression: an example

actual function: $f(x) = x^3 - x^2$

model function: $f(x) = \sum_{i=0}^{p} w_i x^i$



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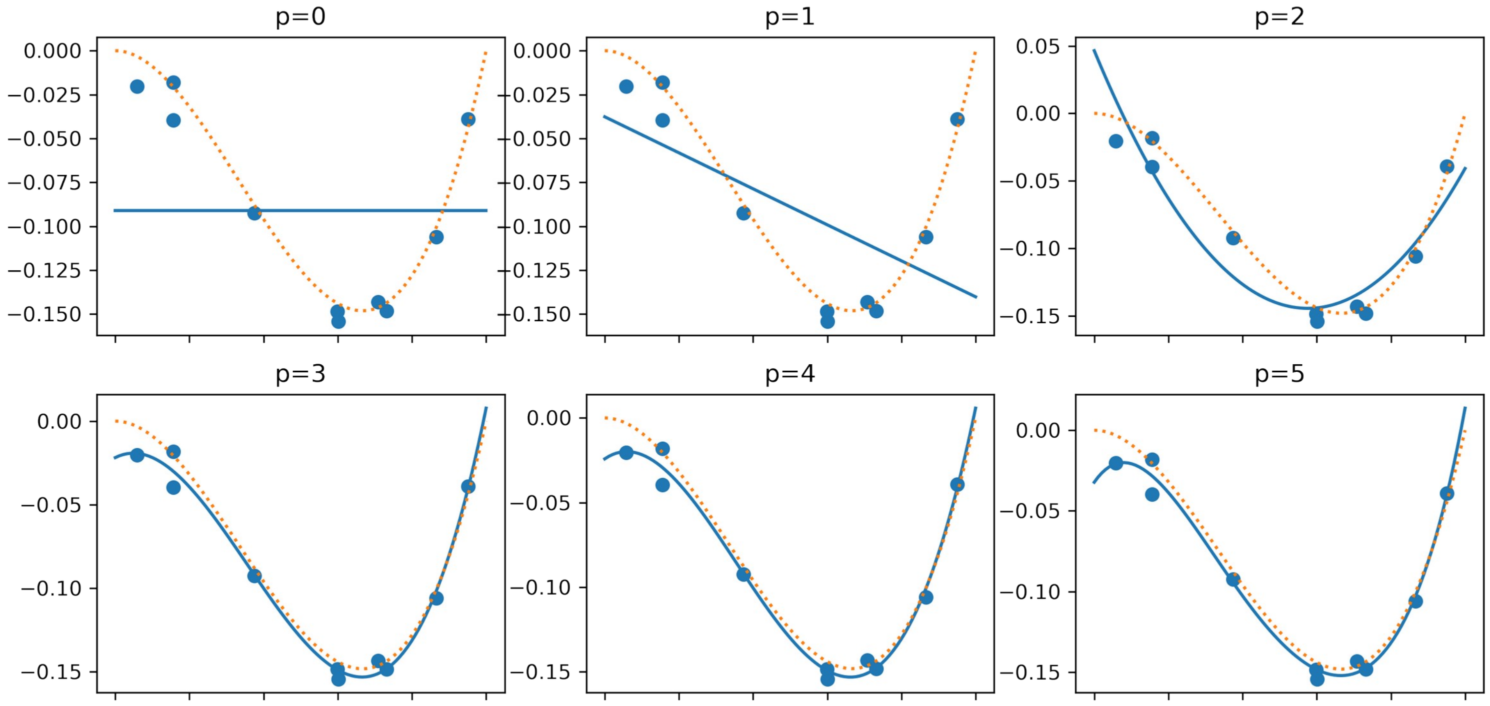

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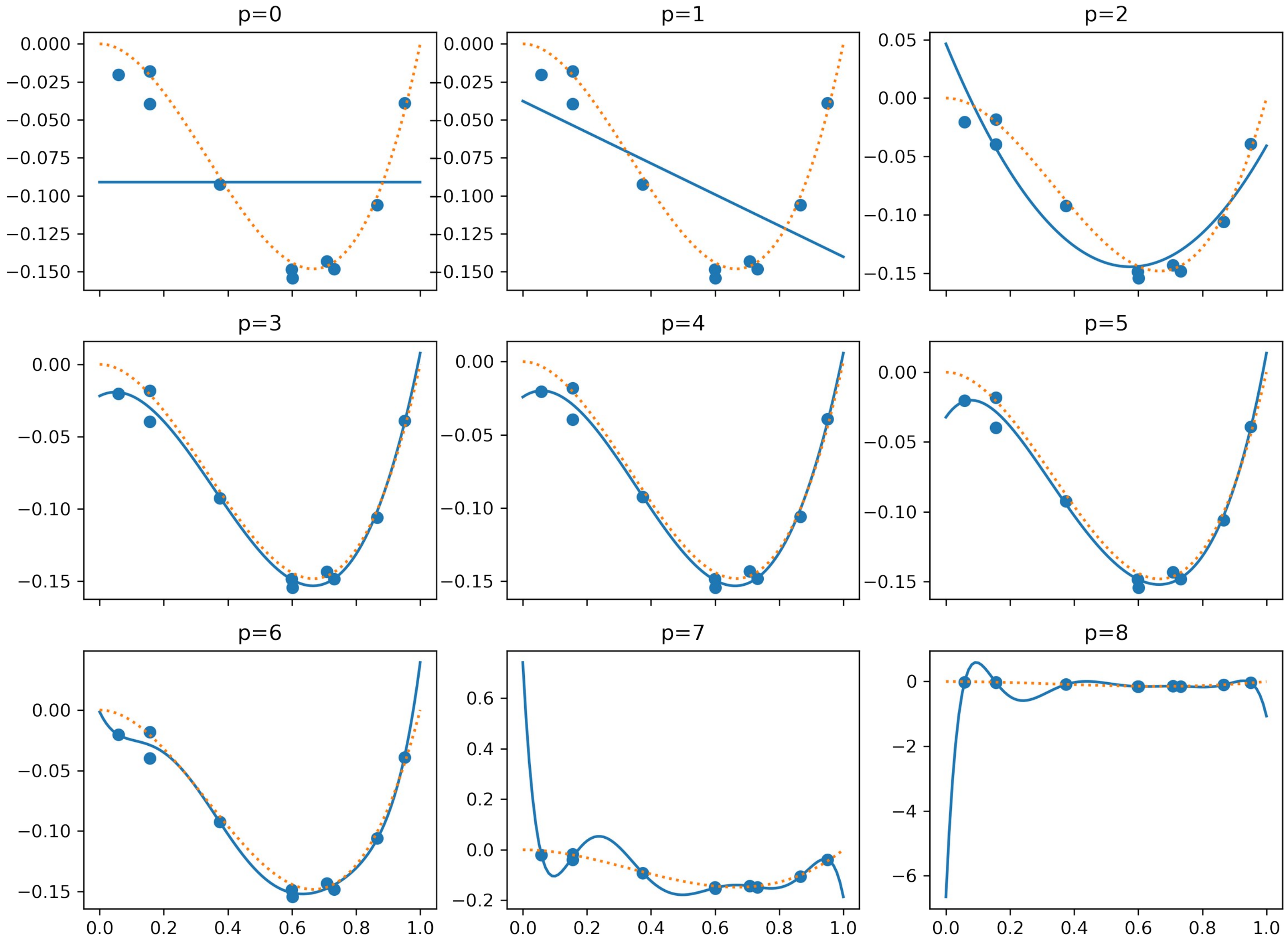

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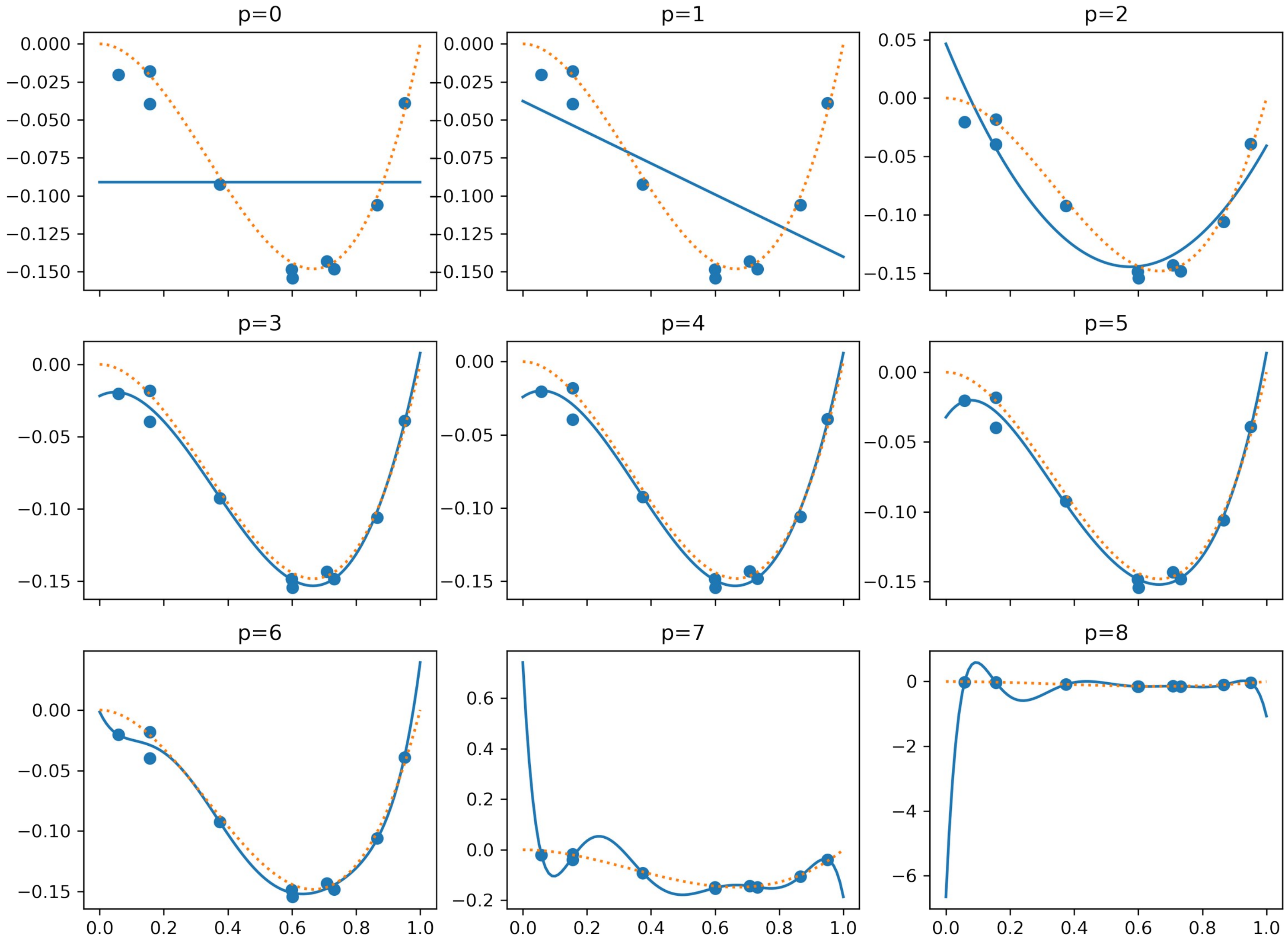

Which model is the best (qualitatively)?

Interlude: Occam's Razor

With competing theories or explanations, the simpler one, for example a model with fewer parameters, is to be preferred.

Moscarlop @ wikimedia

William of Ockham
(1287 - 1347)

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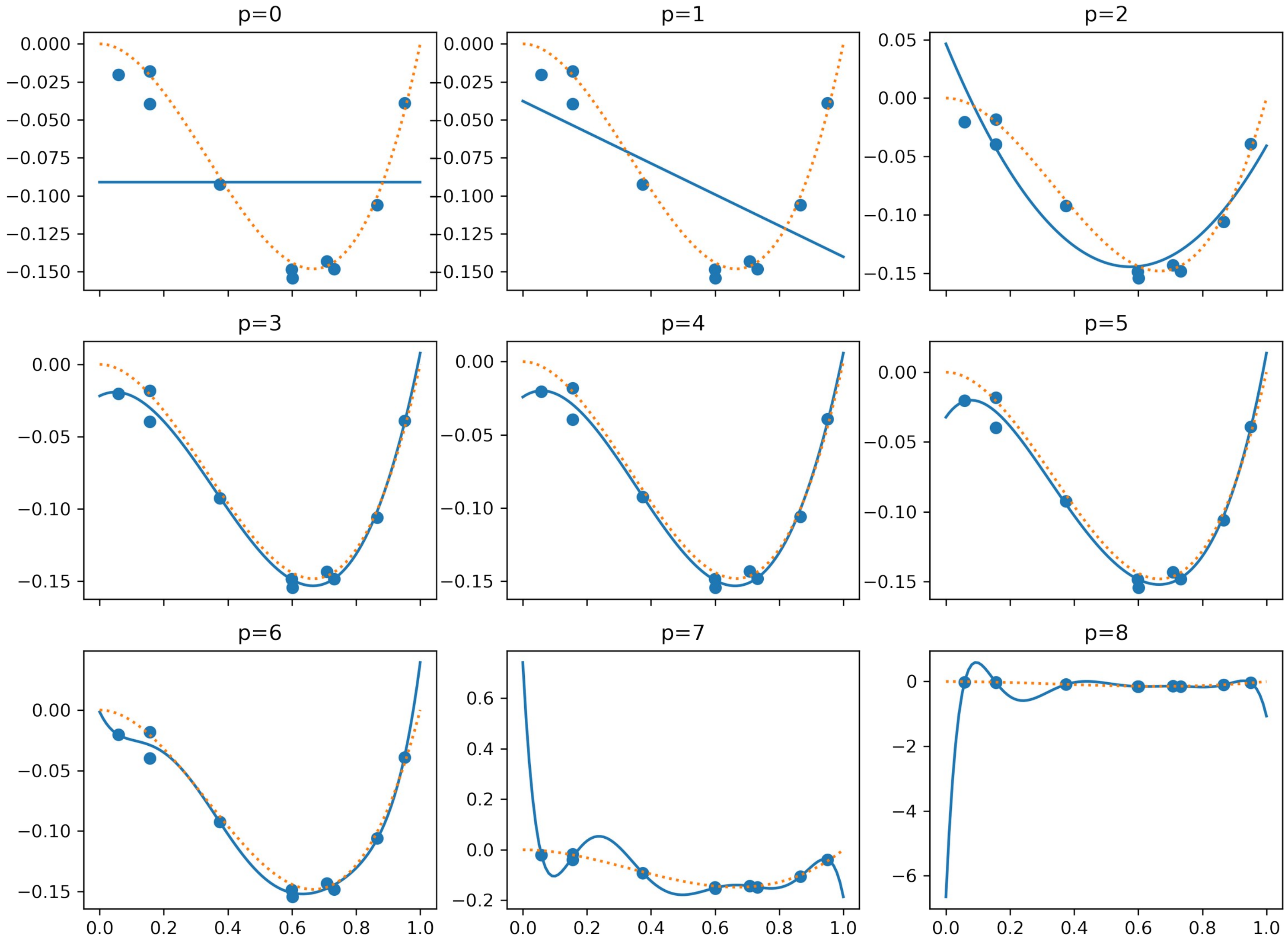

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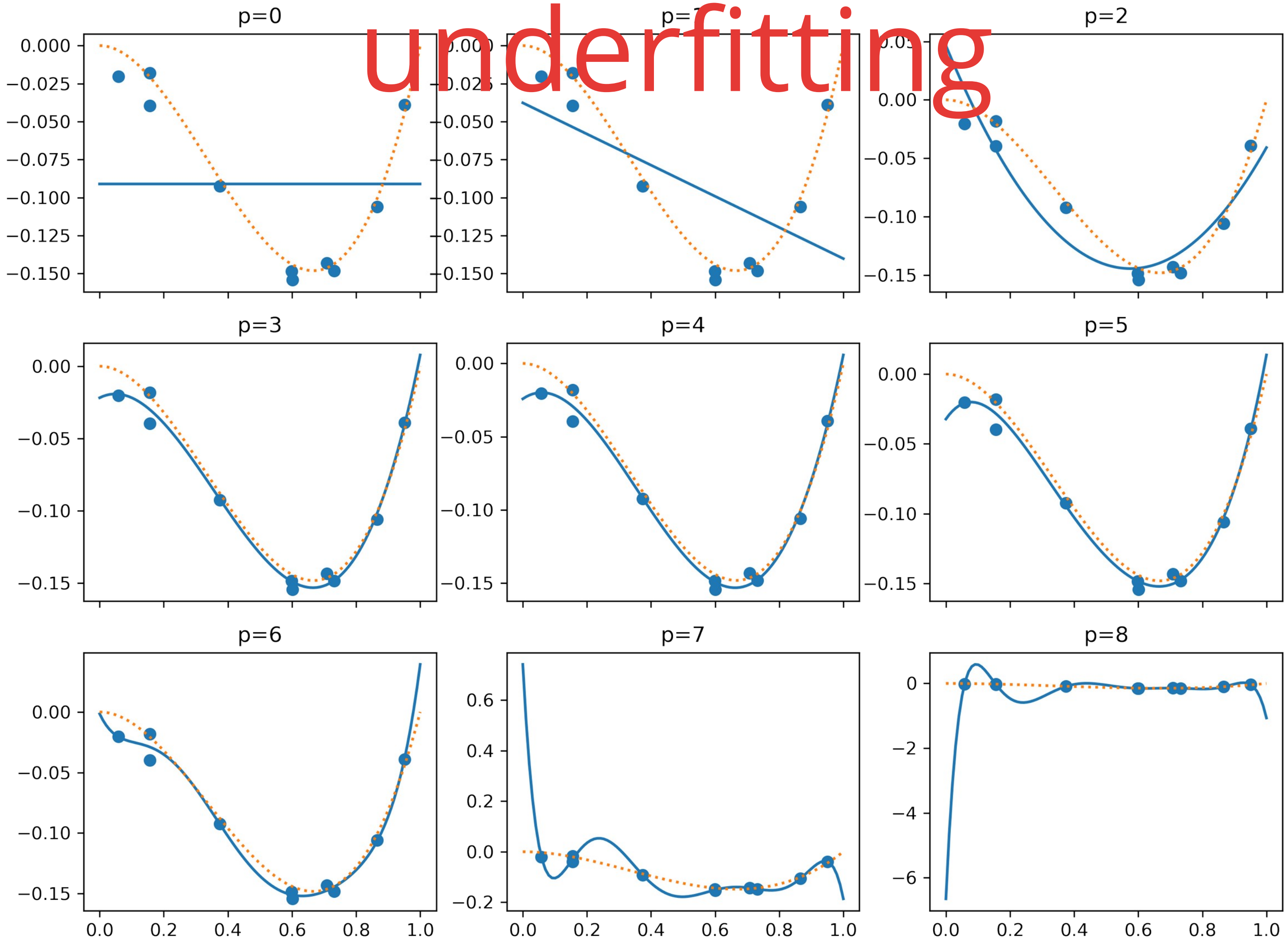
underfitting



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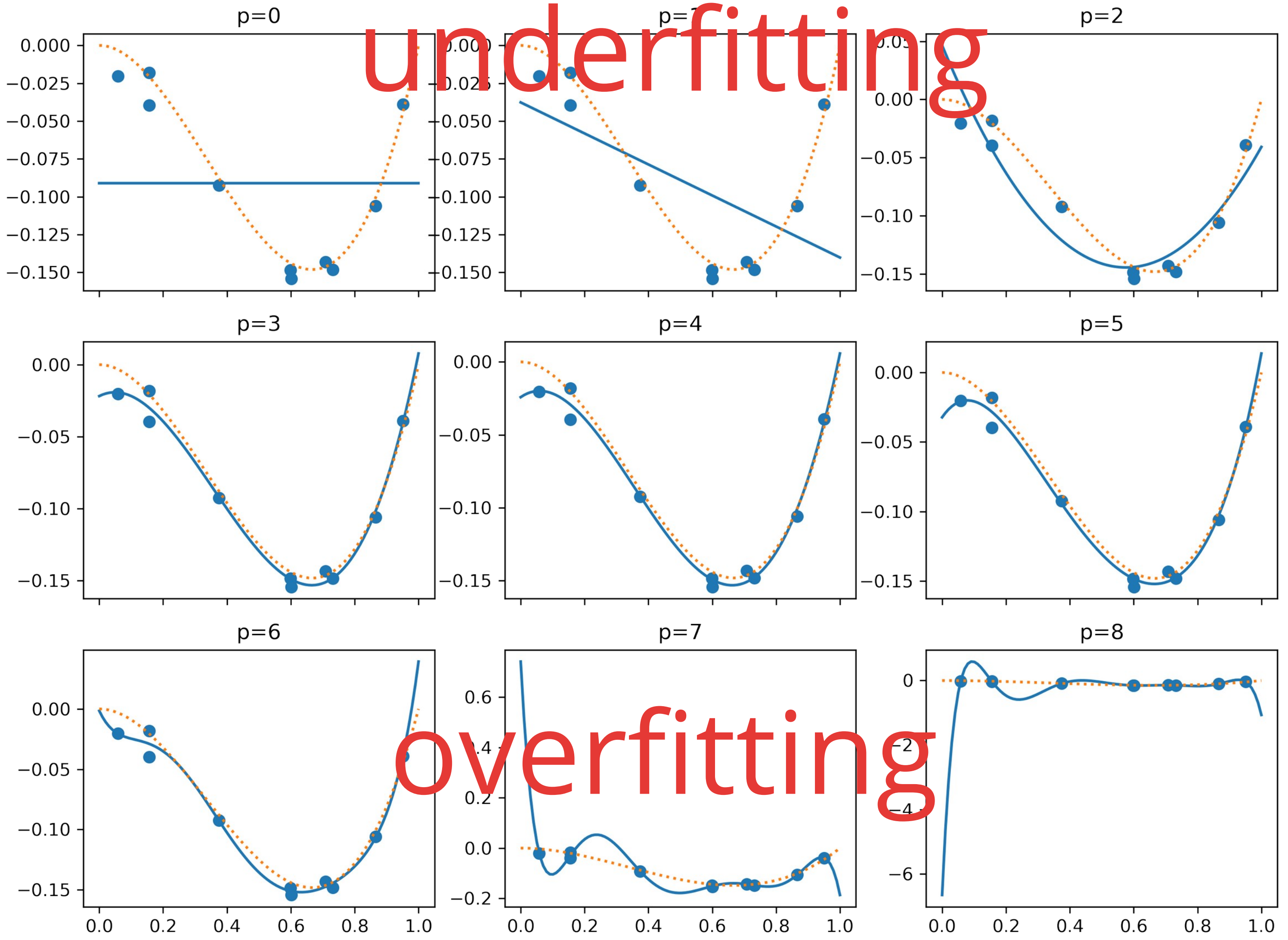

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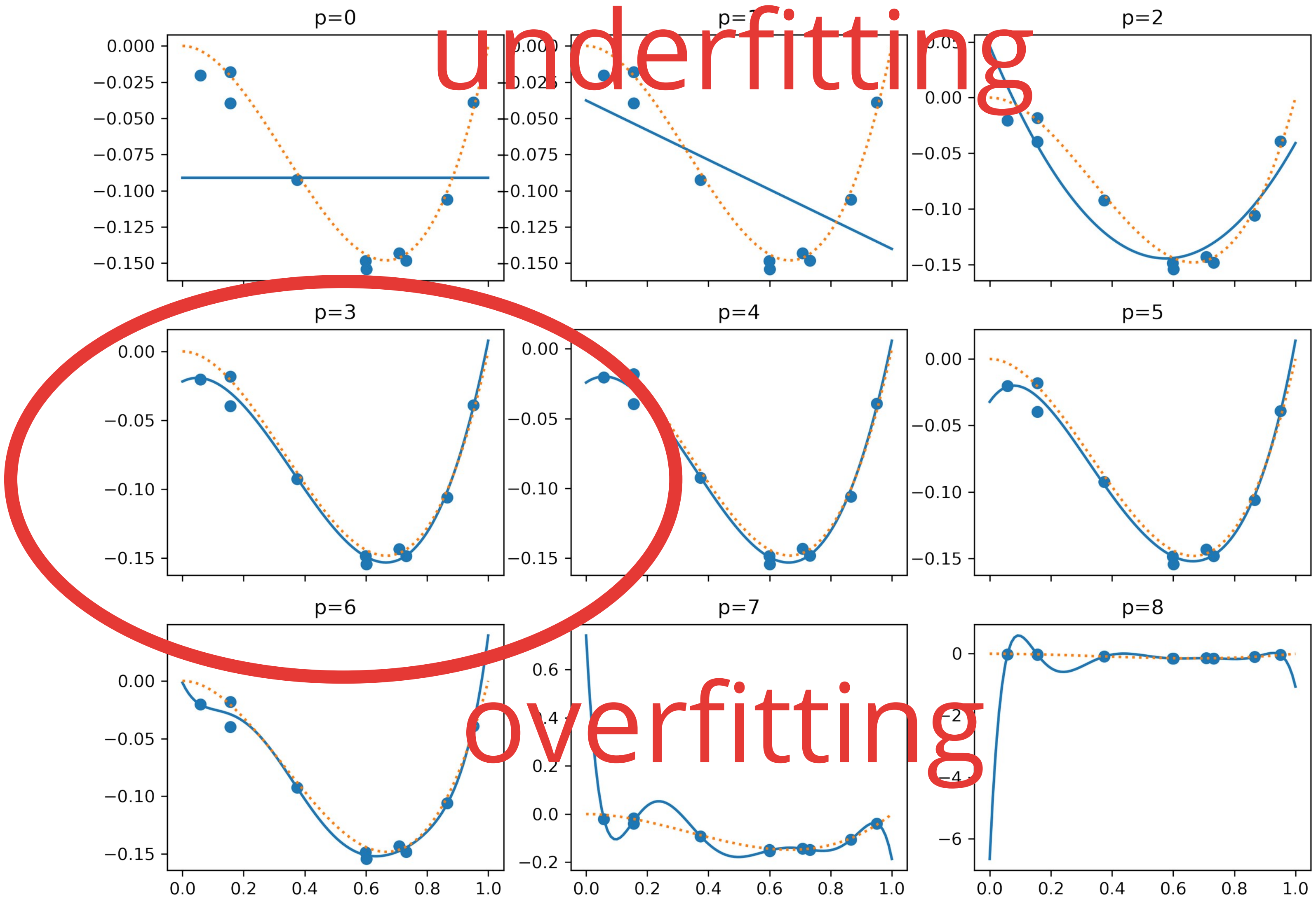

Which model is the best (qualitatively)?

Occam's razor: $p=3$

Polynomial regression: an example

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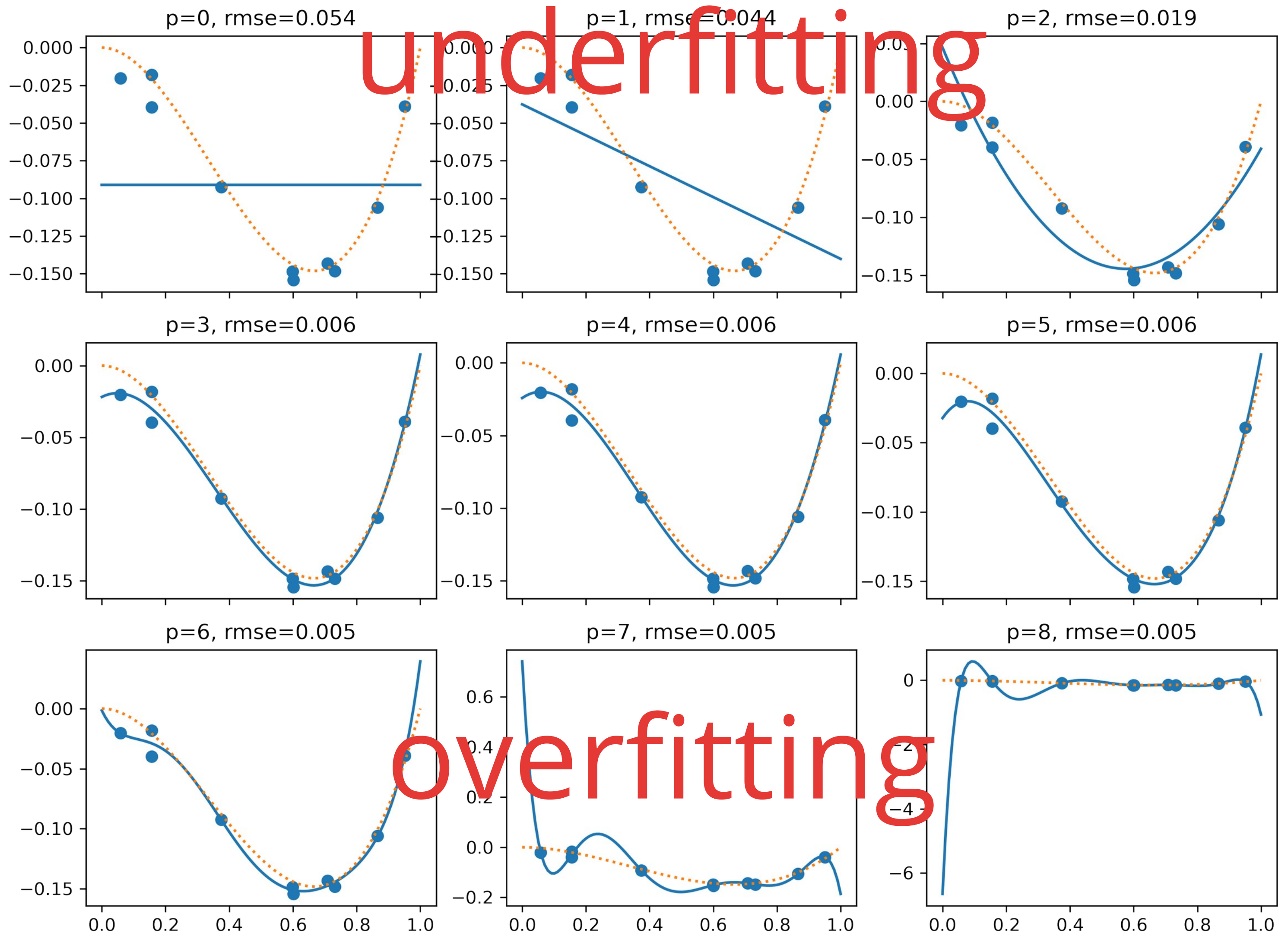

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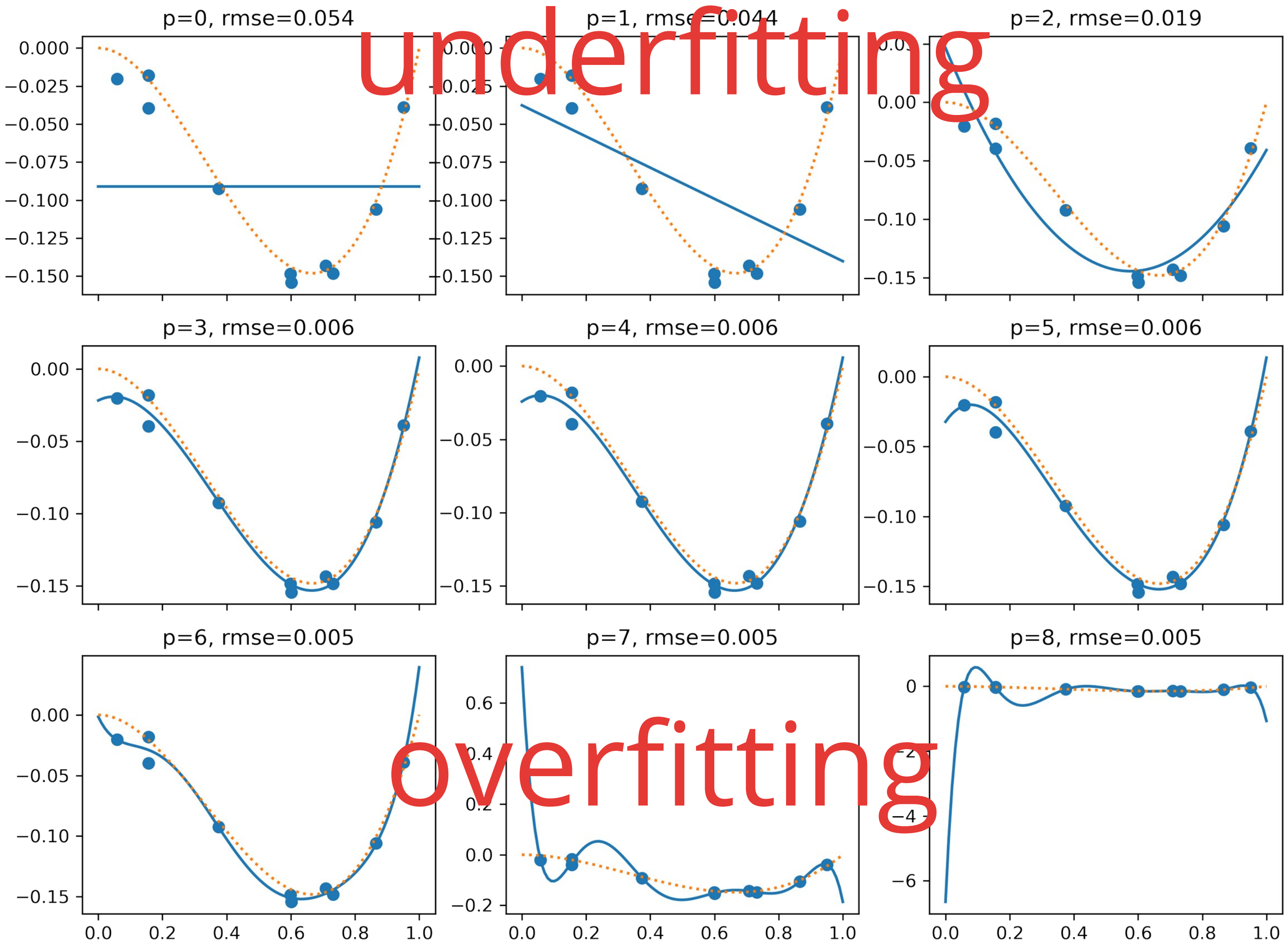

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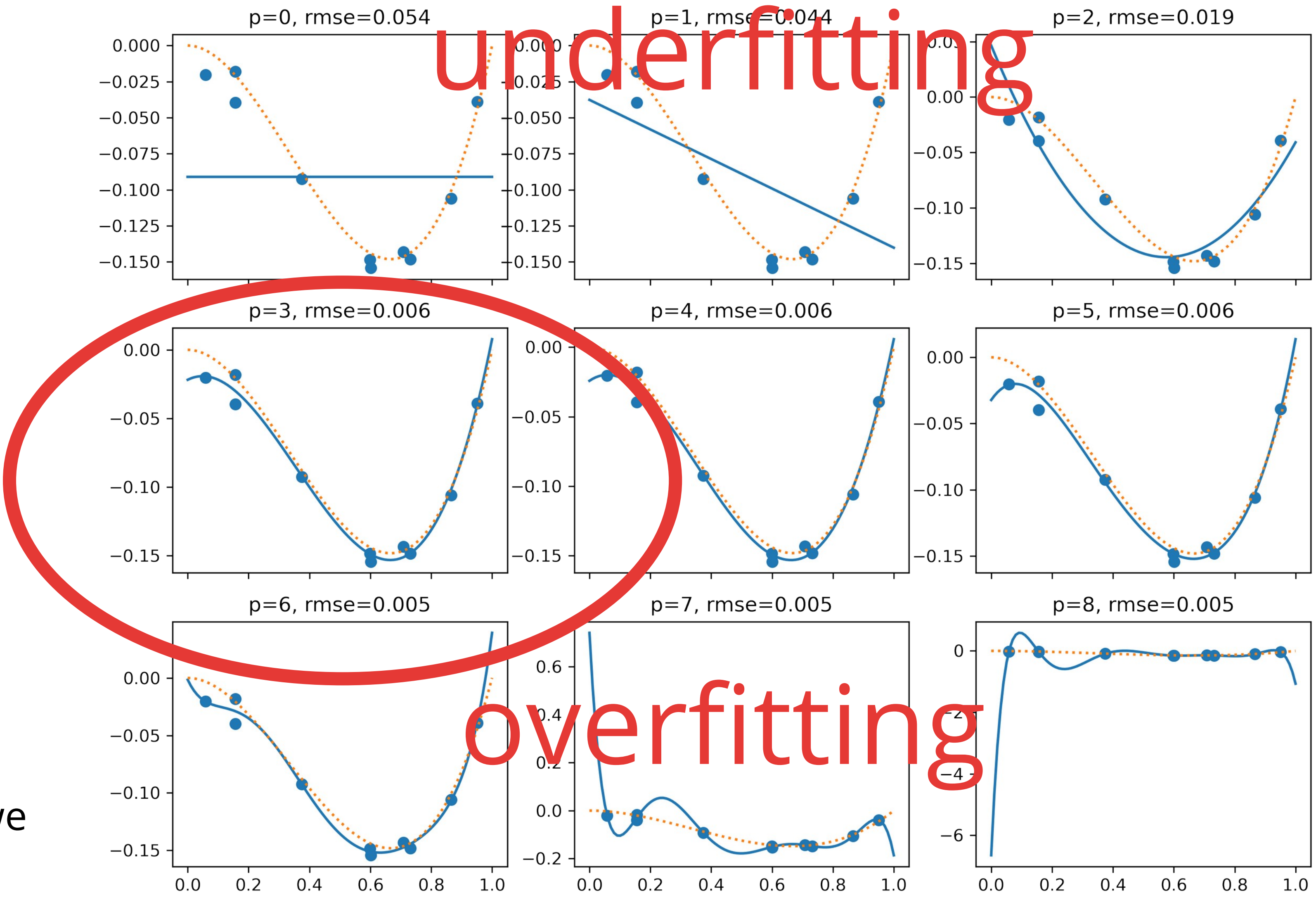

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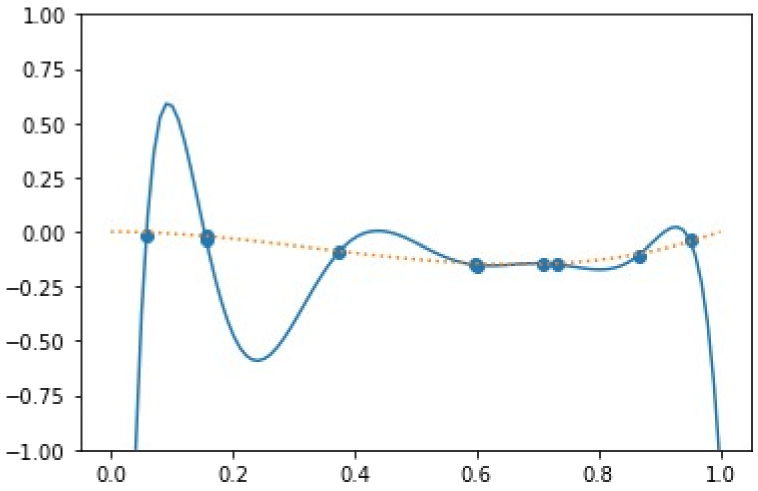

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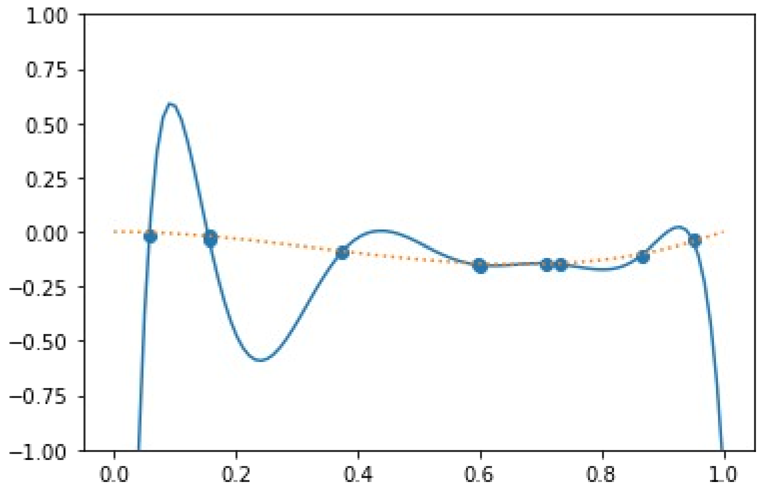

The problem is that the model tries to come as close as possible to the training data to minimize the loss, inevitably **overfitting** and overshooting. We need a way to prevent the model from performing too well on the training data.

L2 regularization: Ridge regression

One way to prevent the model from “doing too well” is to **regularize the loss** based on the learned weights:

$$L'(\boldsymbol{x}, \boldsymbol{w}) = \frac{1}{N} \sum_{i}^{N} L_i(f(\boldsymbol{x_i}, \boldsymbol{w}), \boldsymbol{y_i}) + \alpha \|\boldsymbol{w}\|_2^2$$

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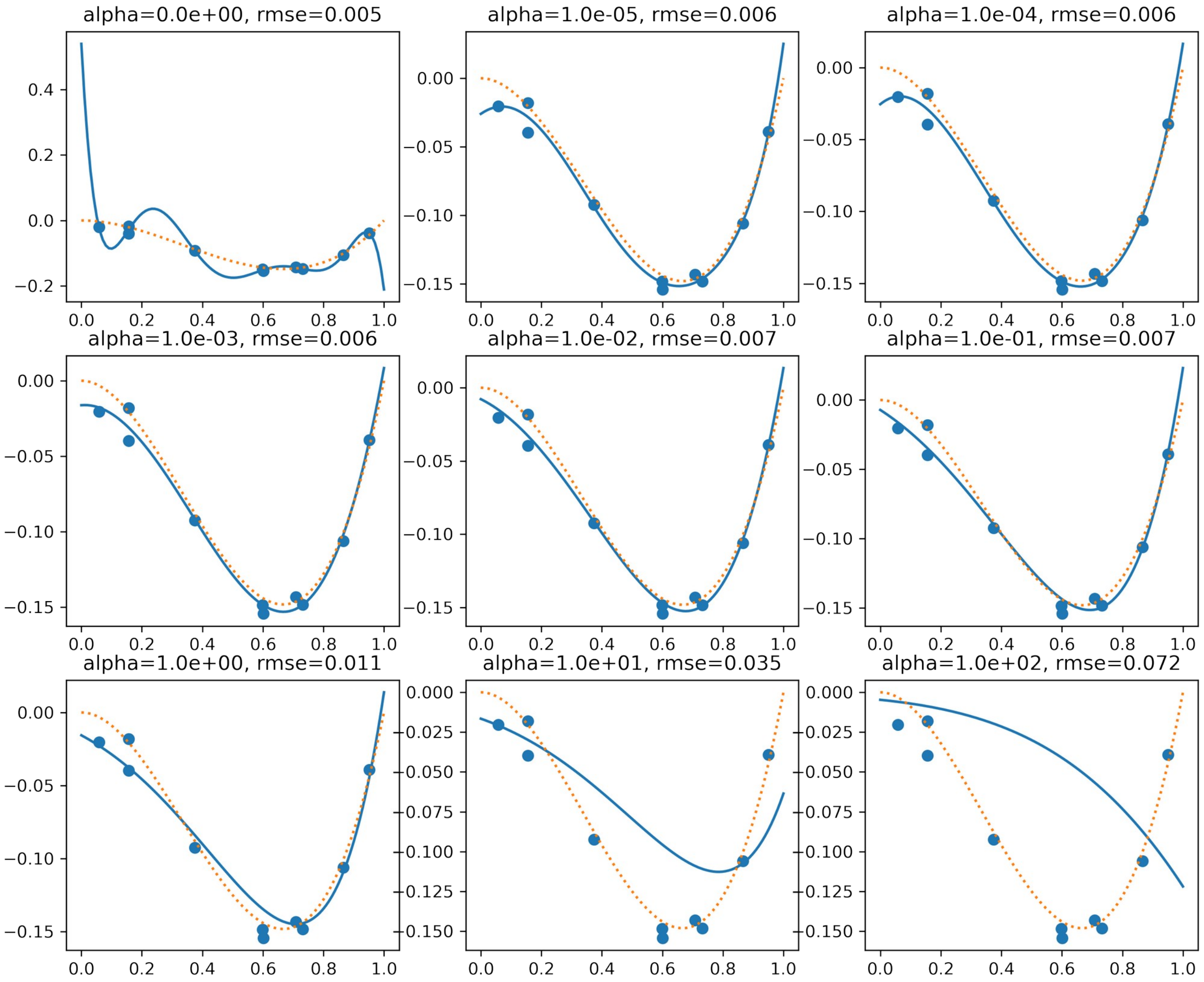

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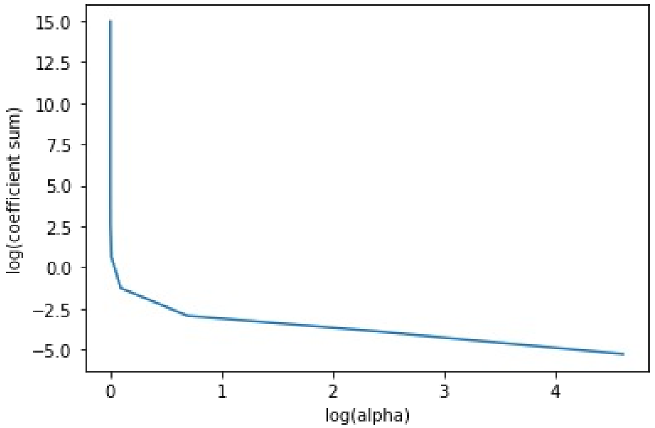

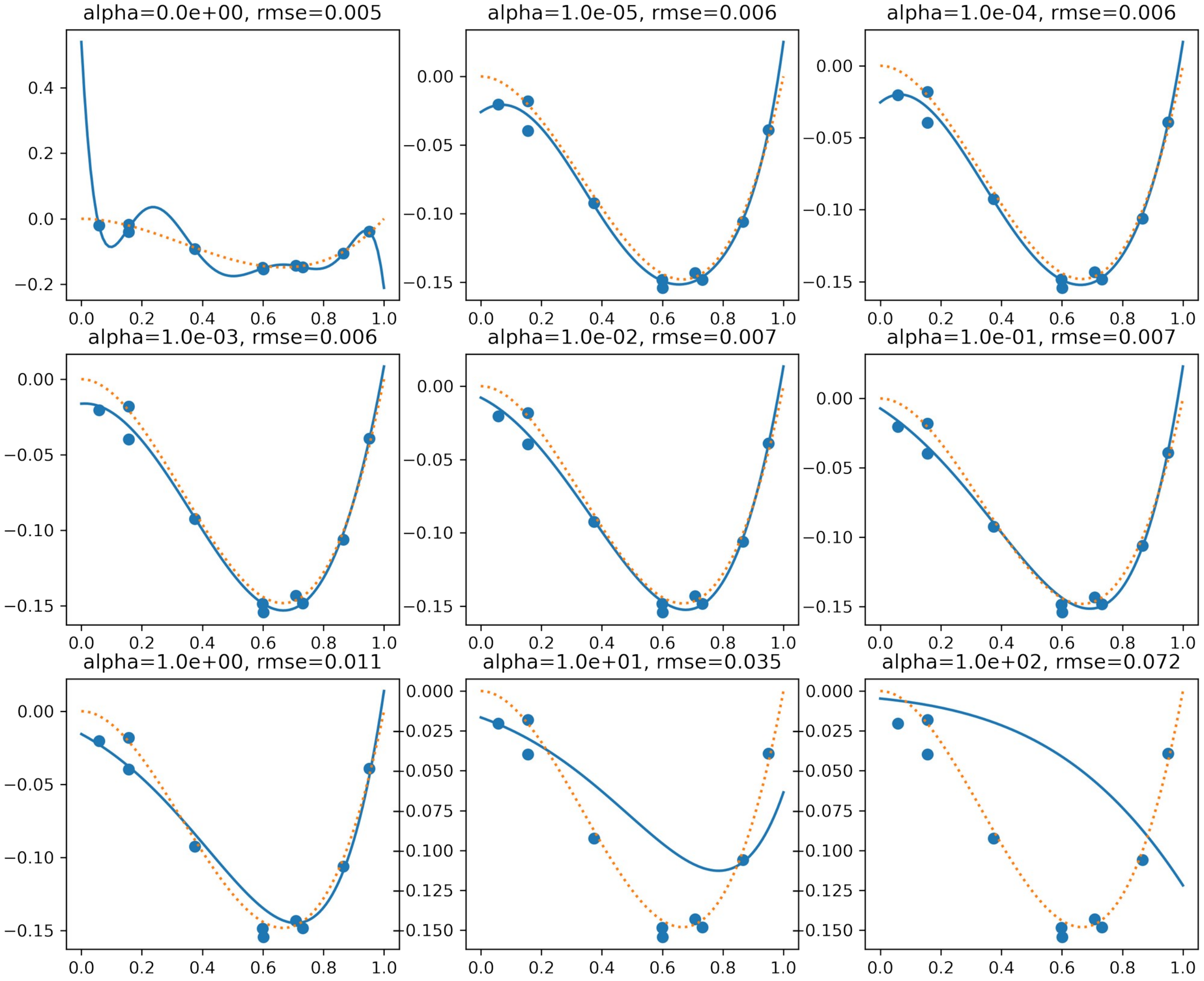

With increasing alpha, all coefficients w_i drop in magnitude, leading to smoother fits → **regularization**

L1 regularization: LASSO regression

We can use a different regularization term:

"LASSO": least absolute shrinkage and selection operator

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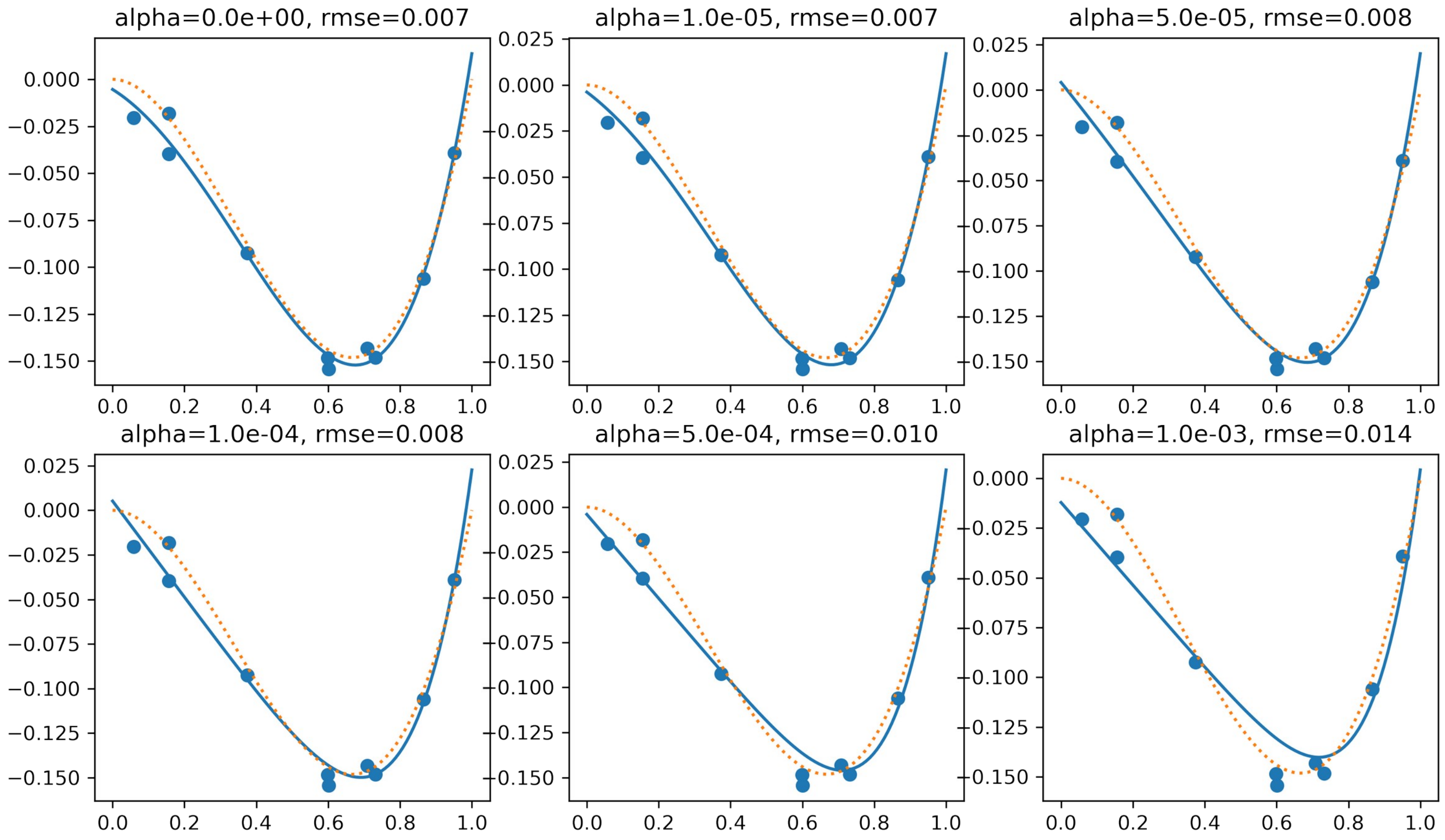

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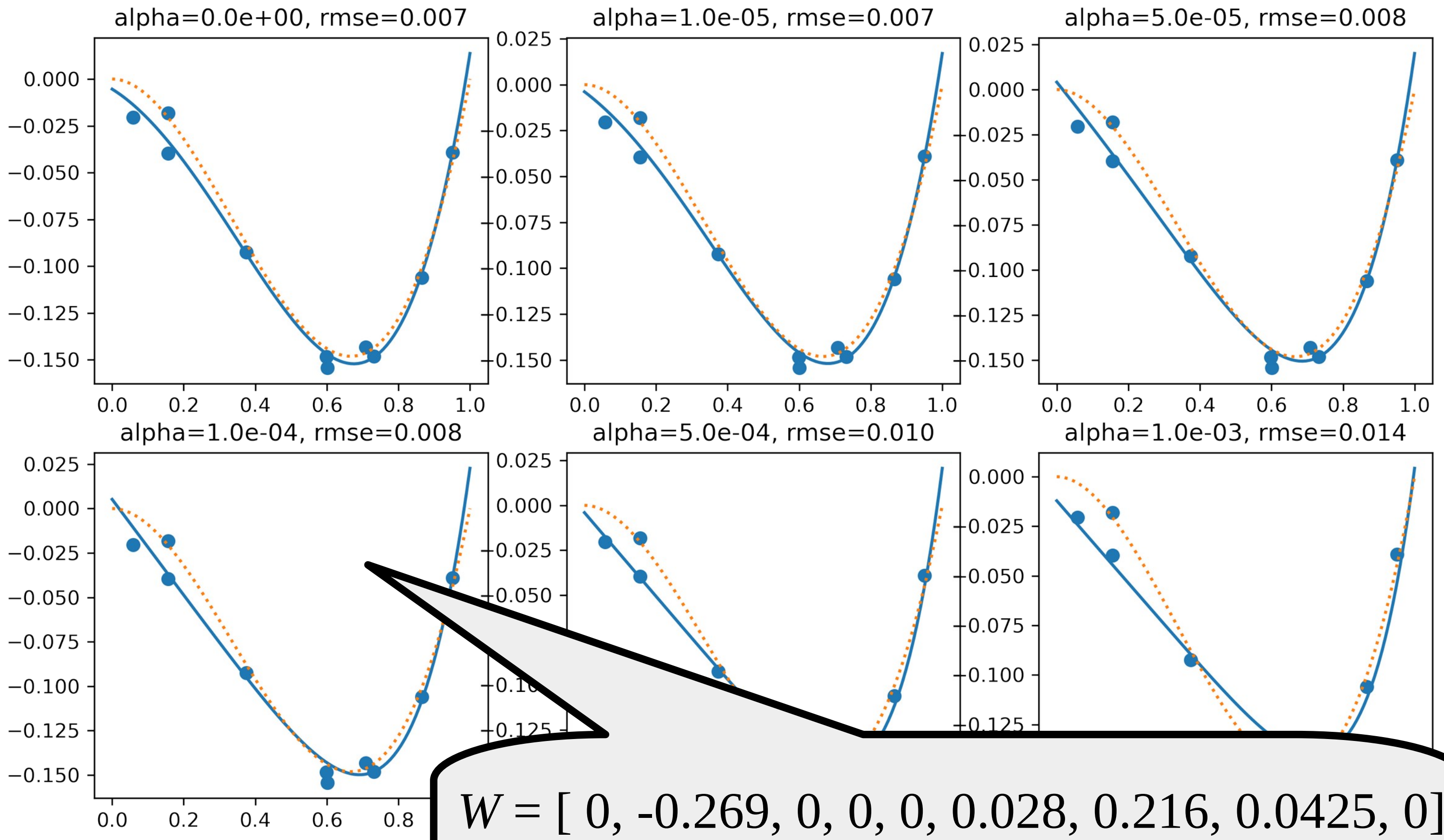

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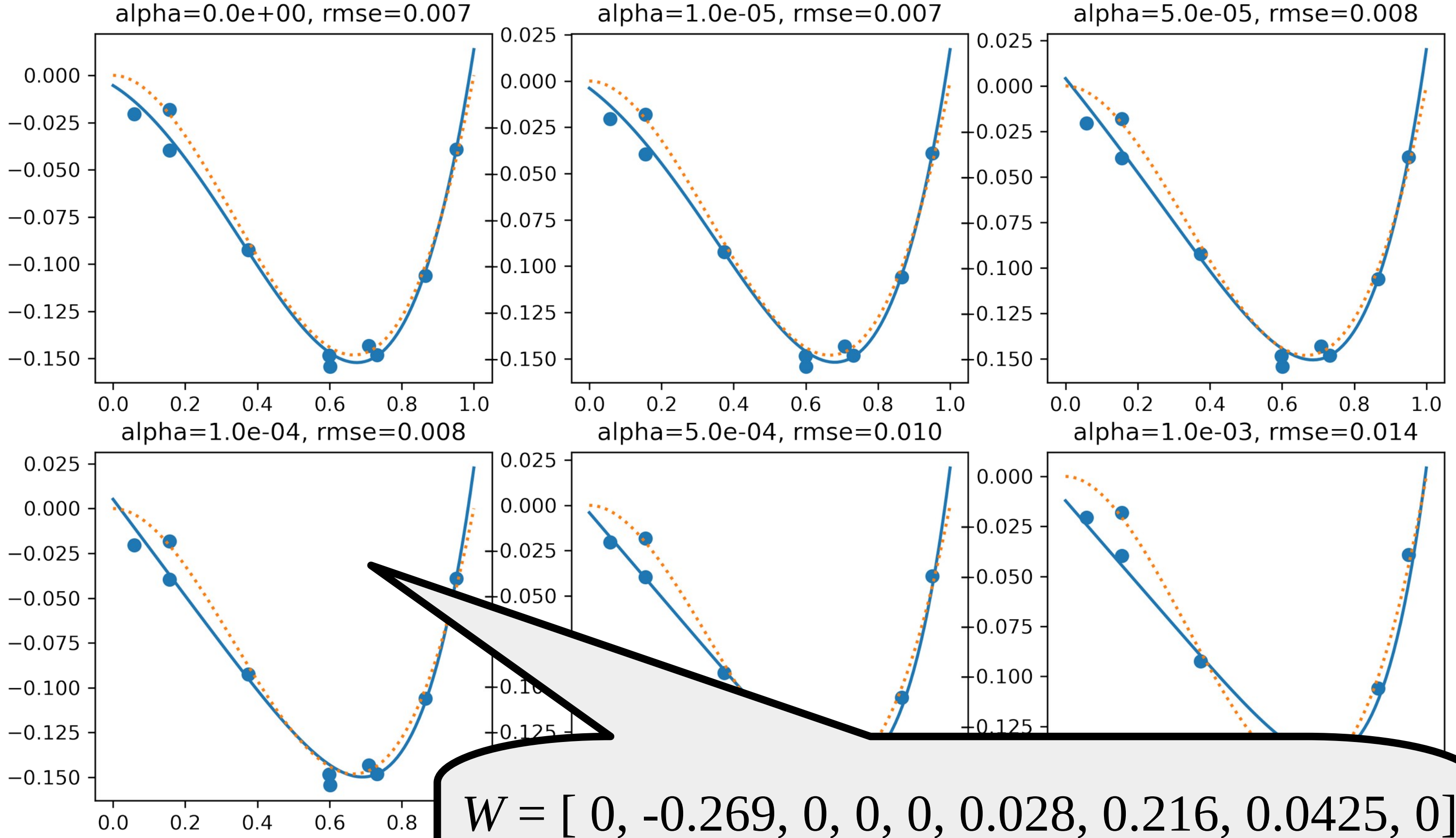

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⇩

$$f(x) = -0.269\,x + 0.028\,x^5 + 0.216\,x^6 + 0.0425\,x^7$$

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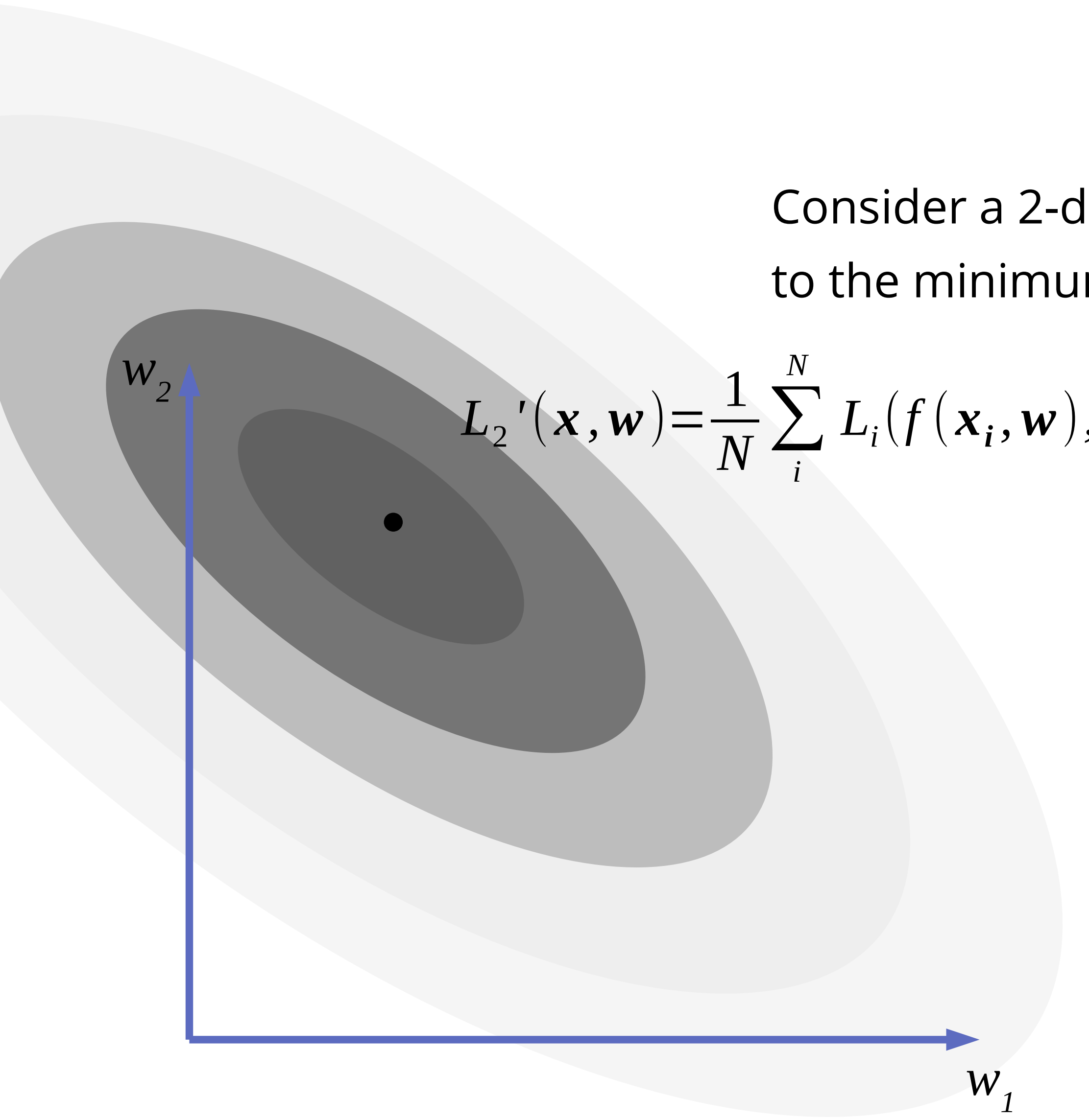

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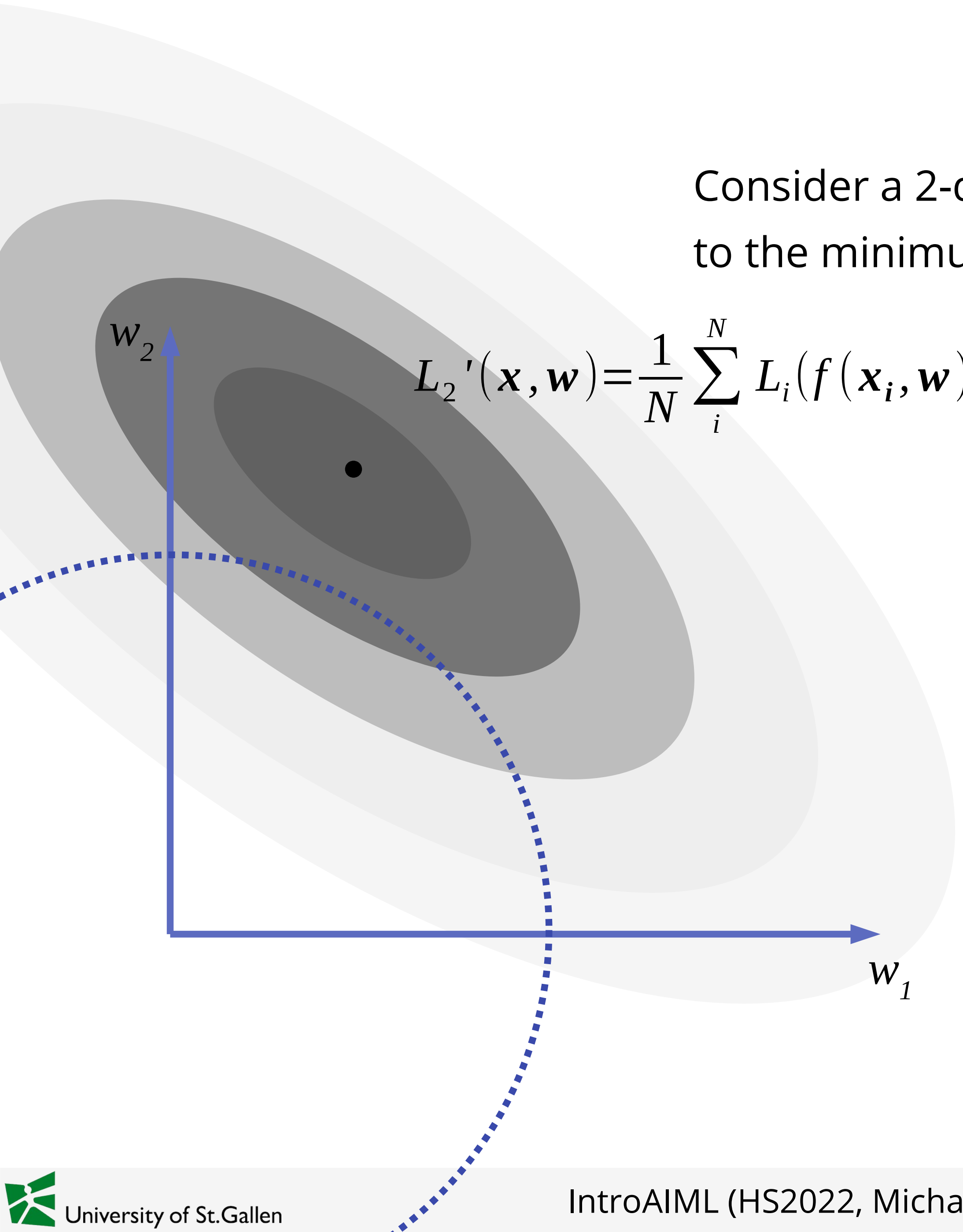

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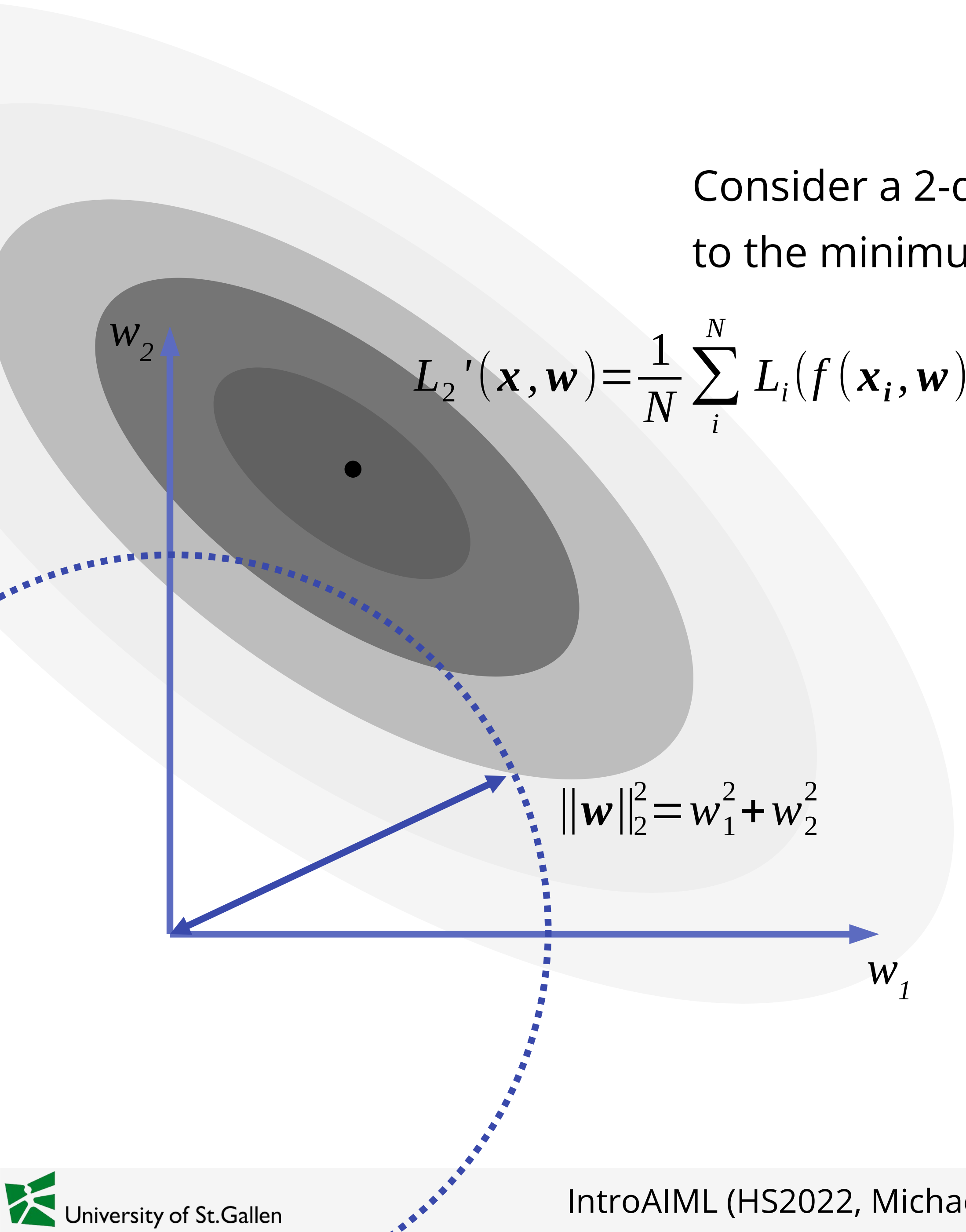

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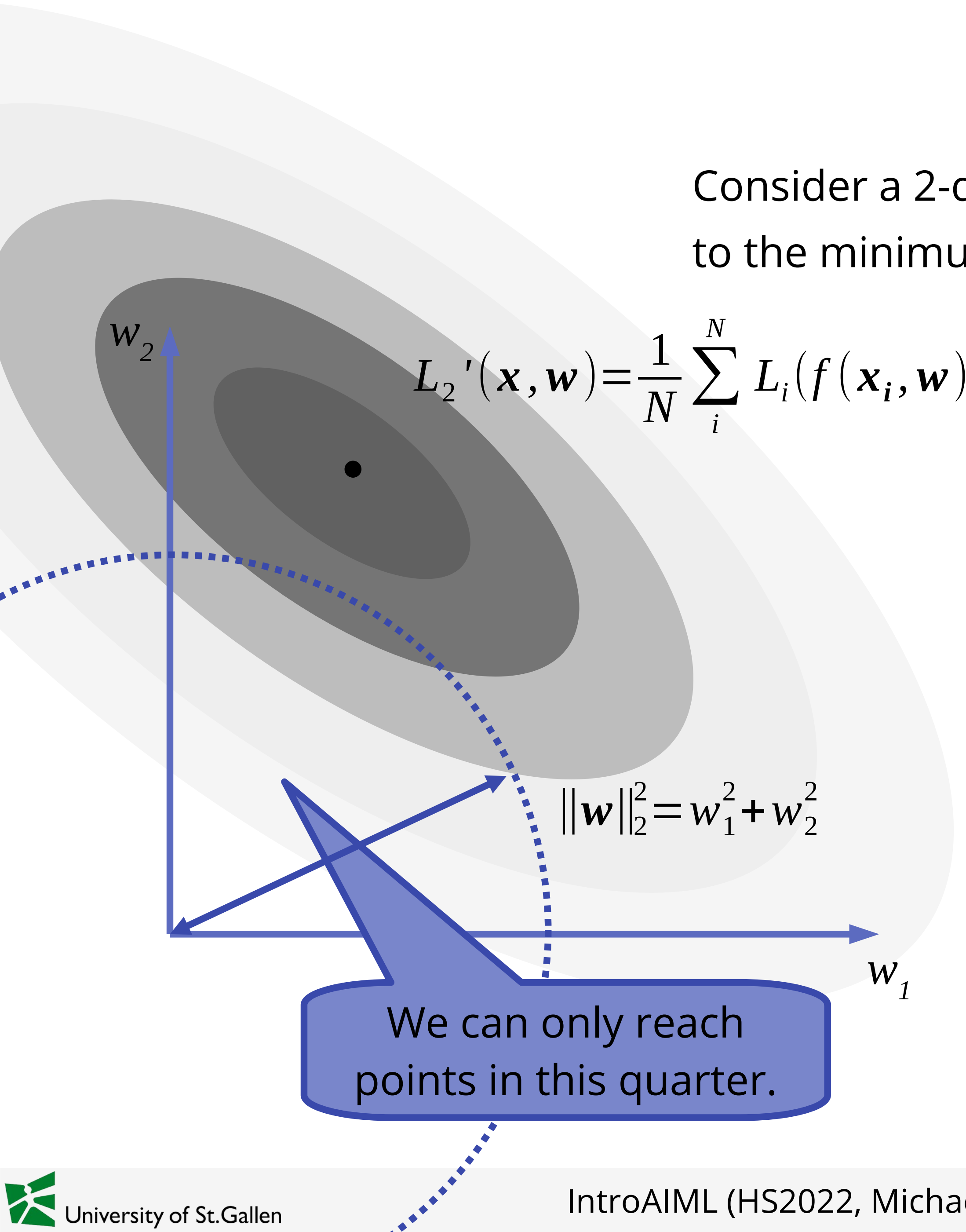

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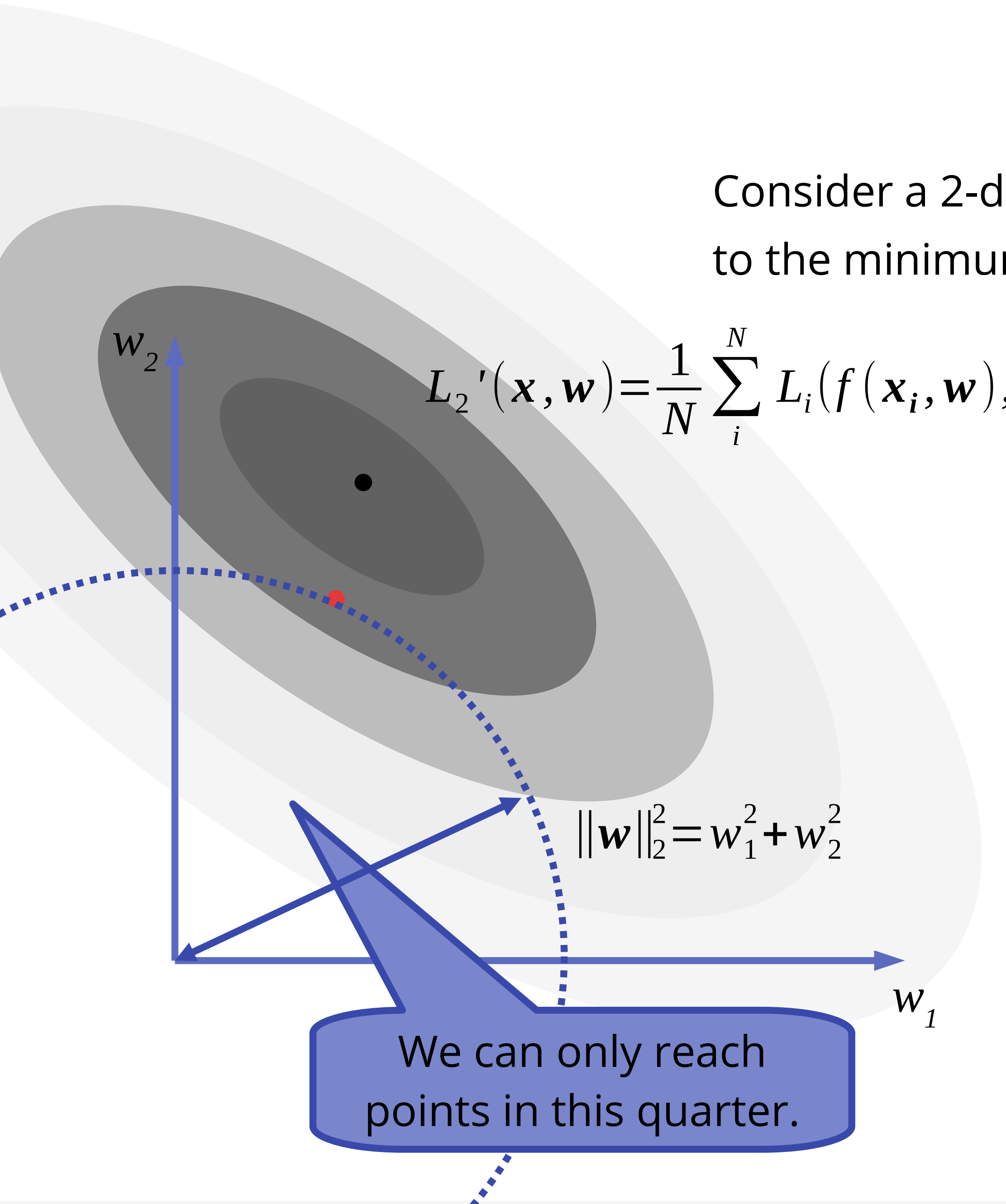

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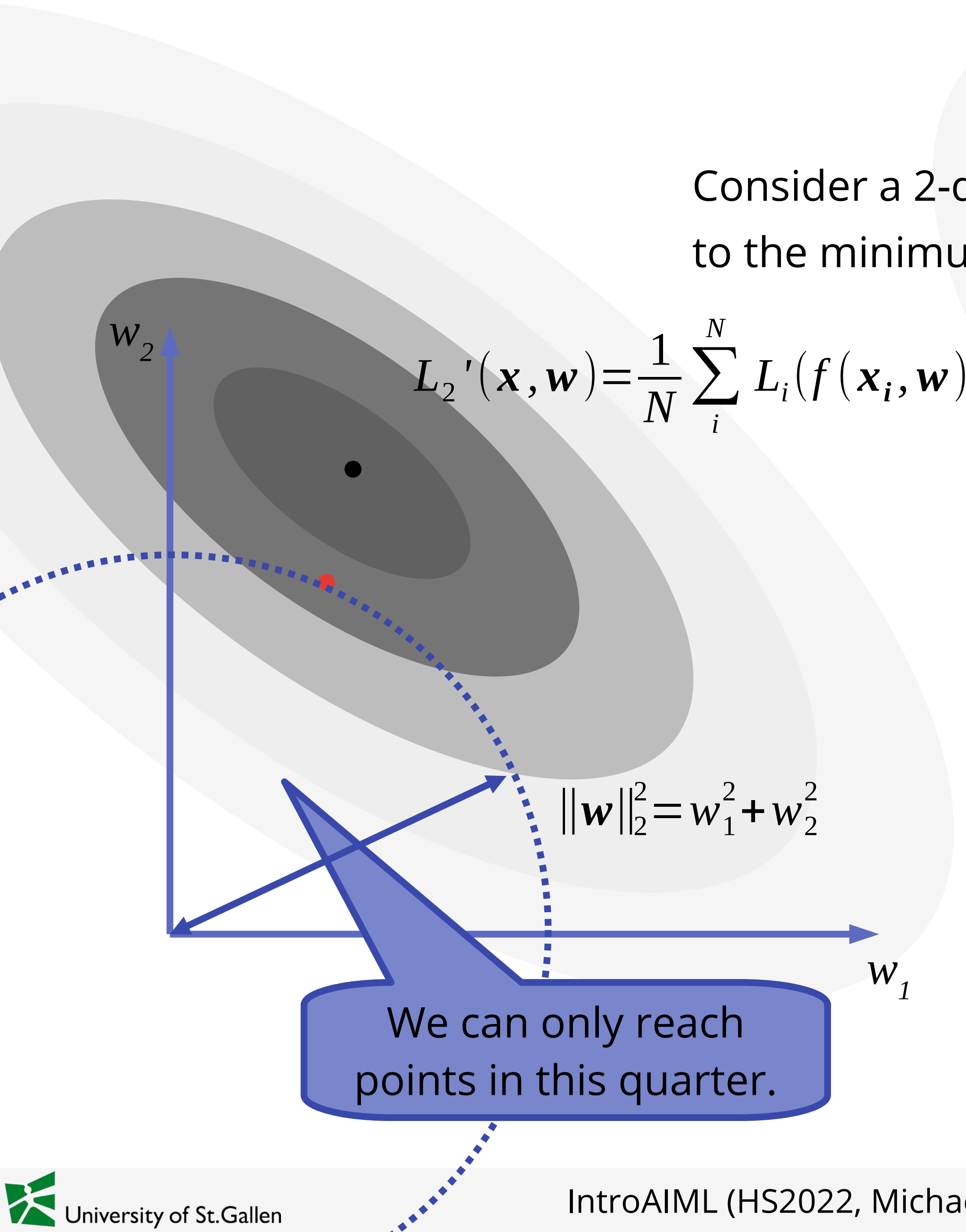

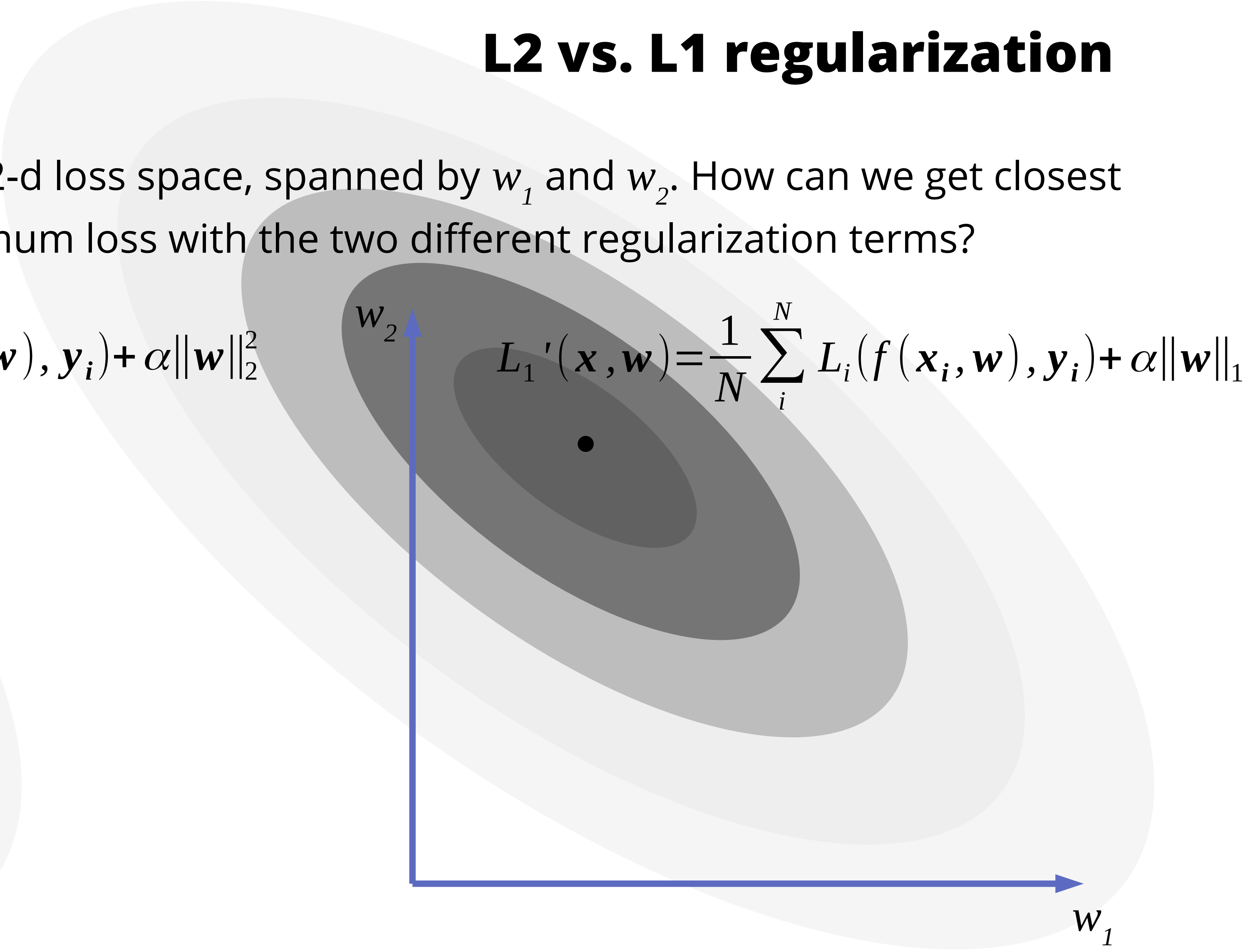

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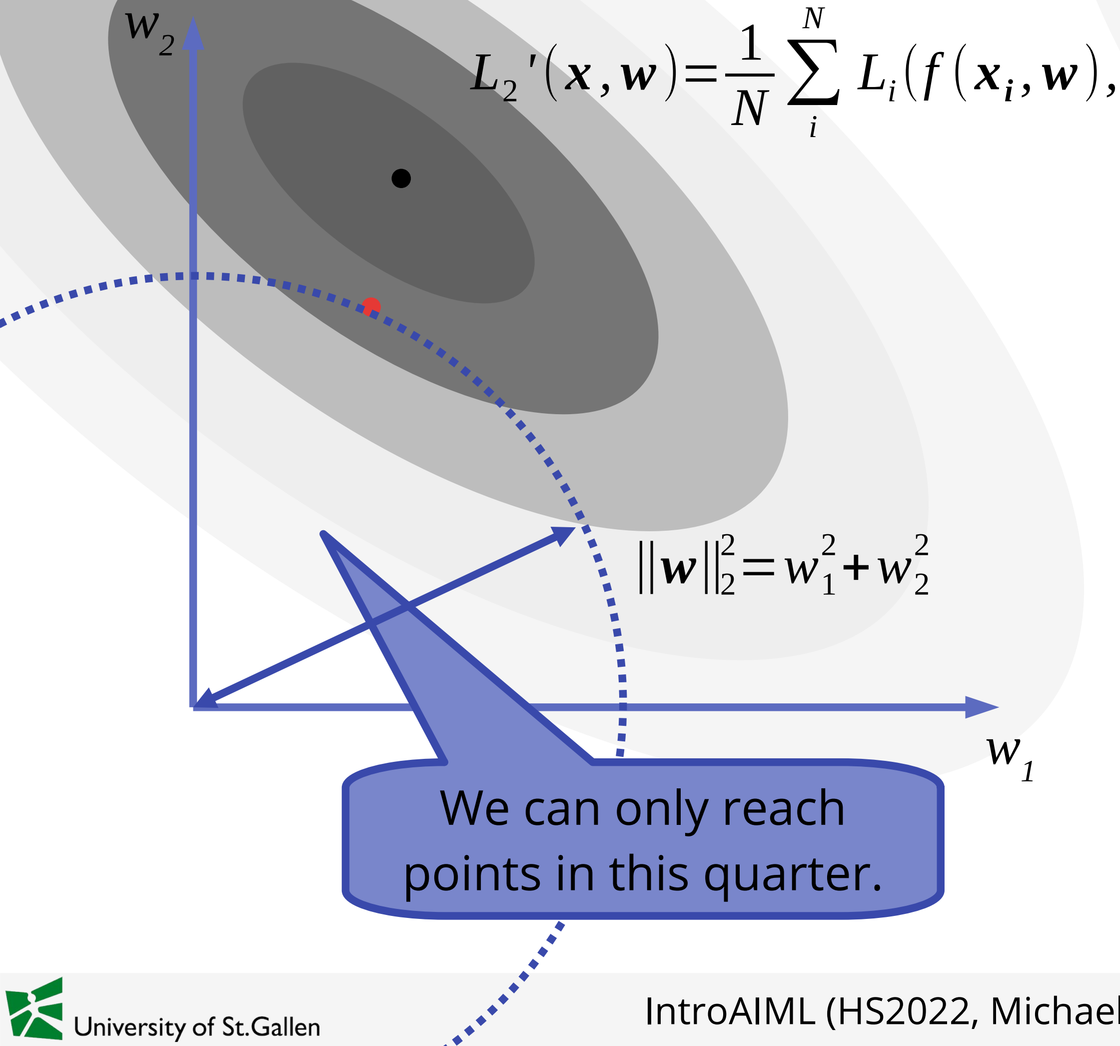

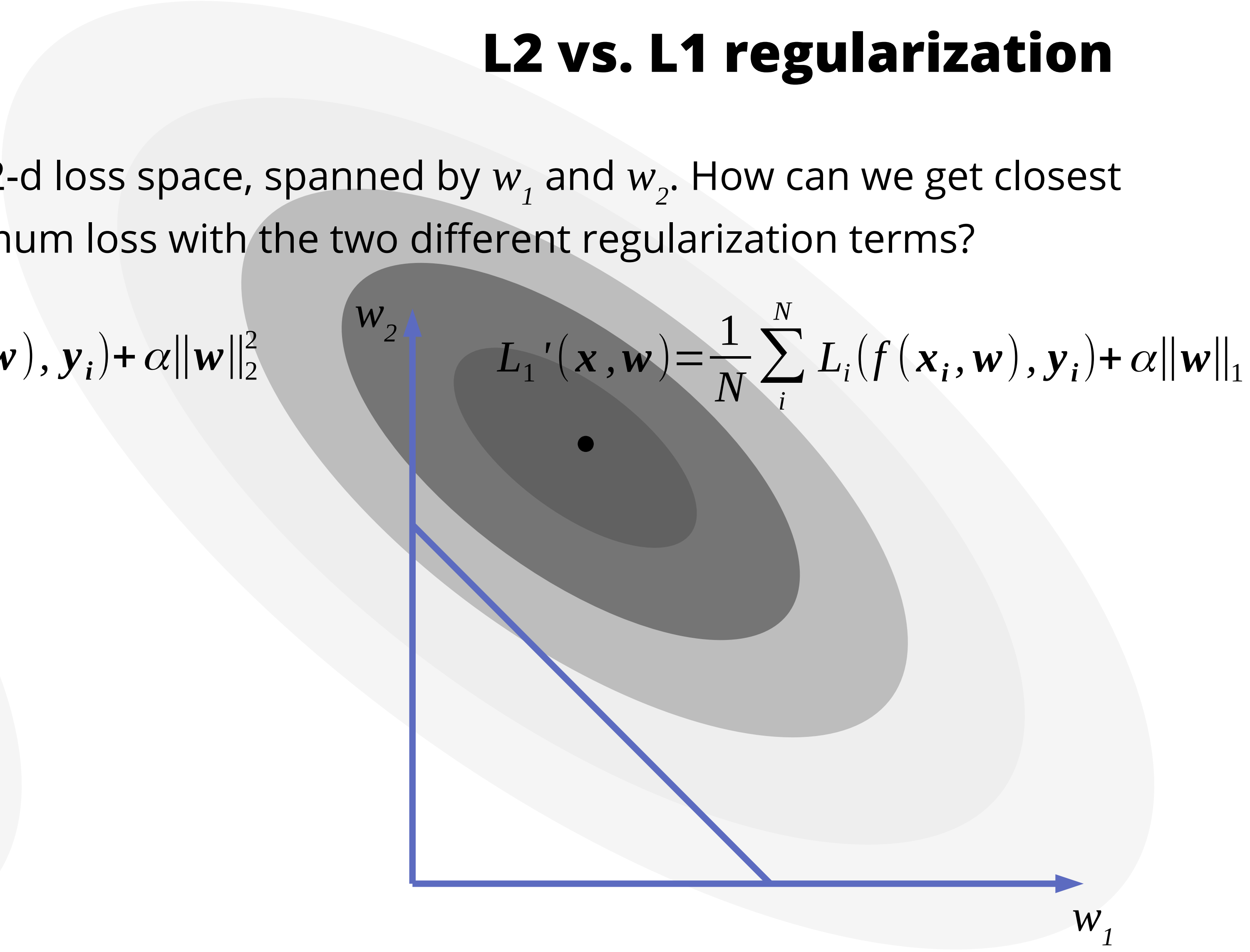

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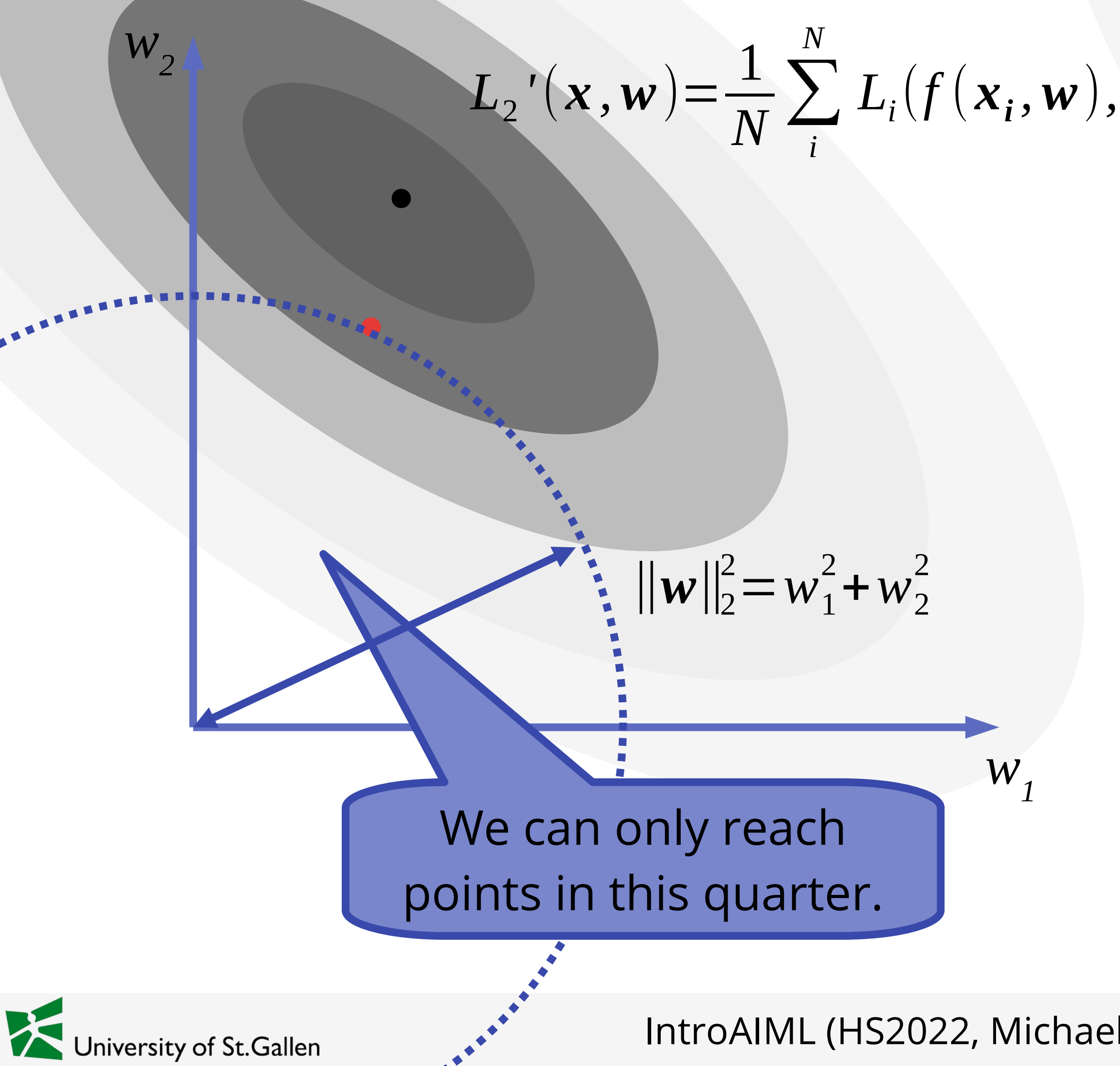

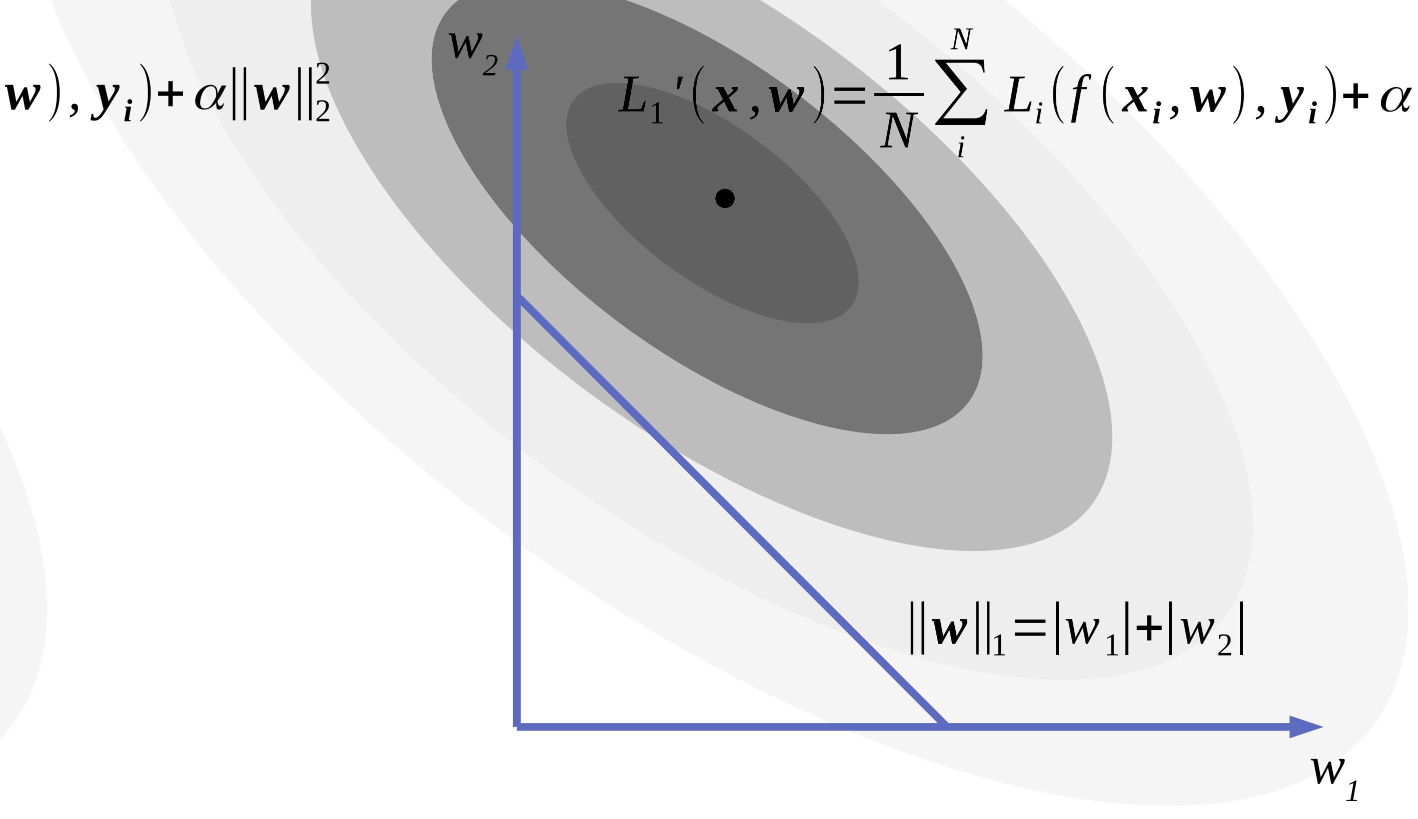

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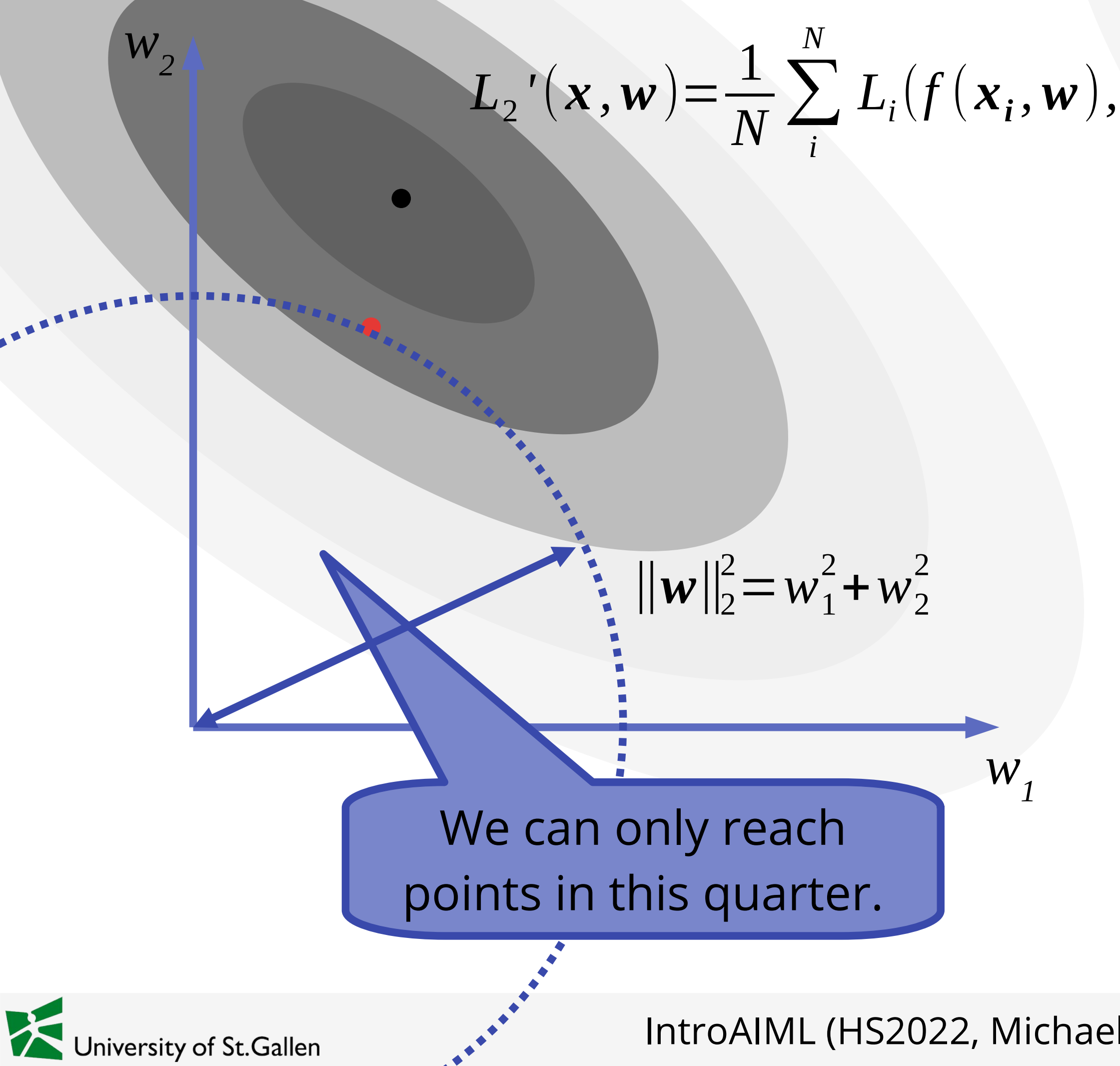

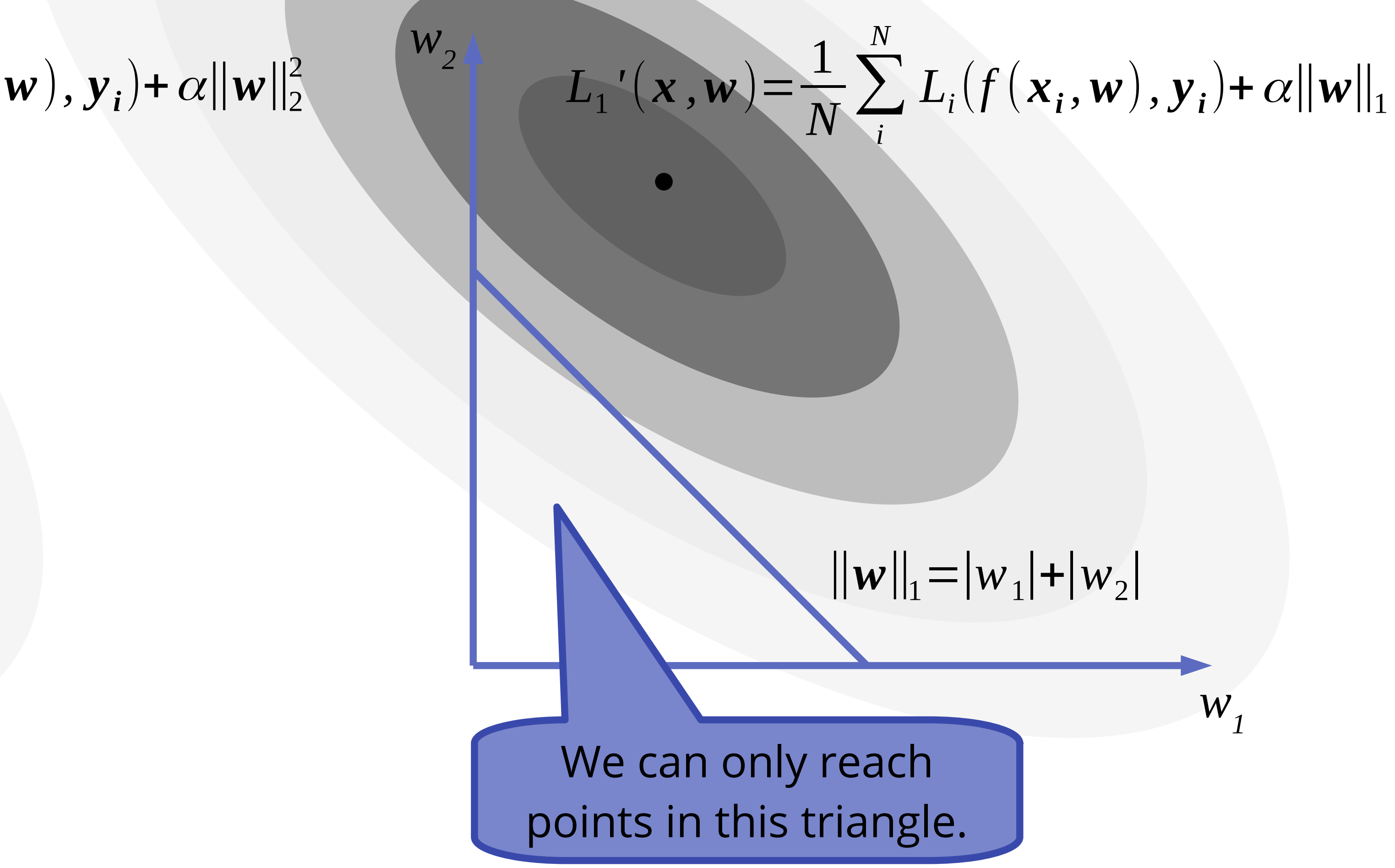

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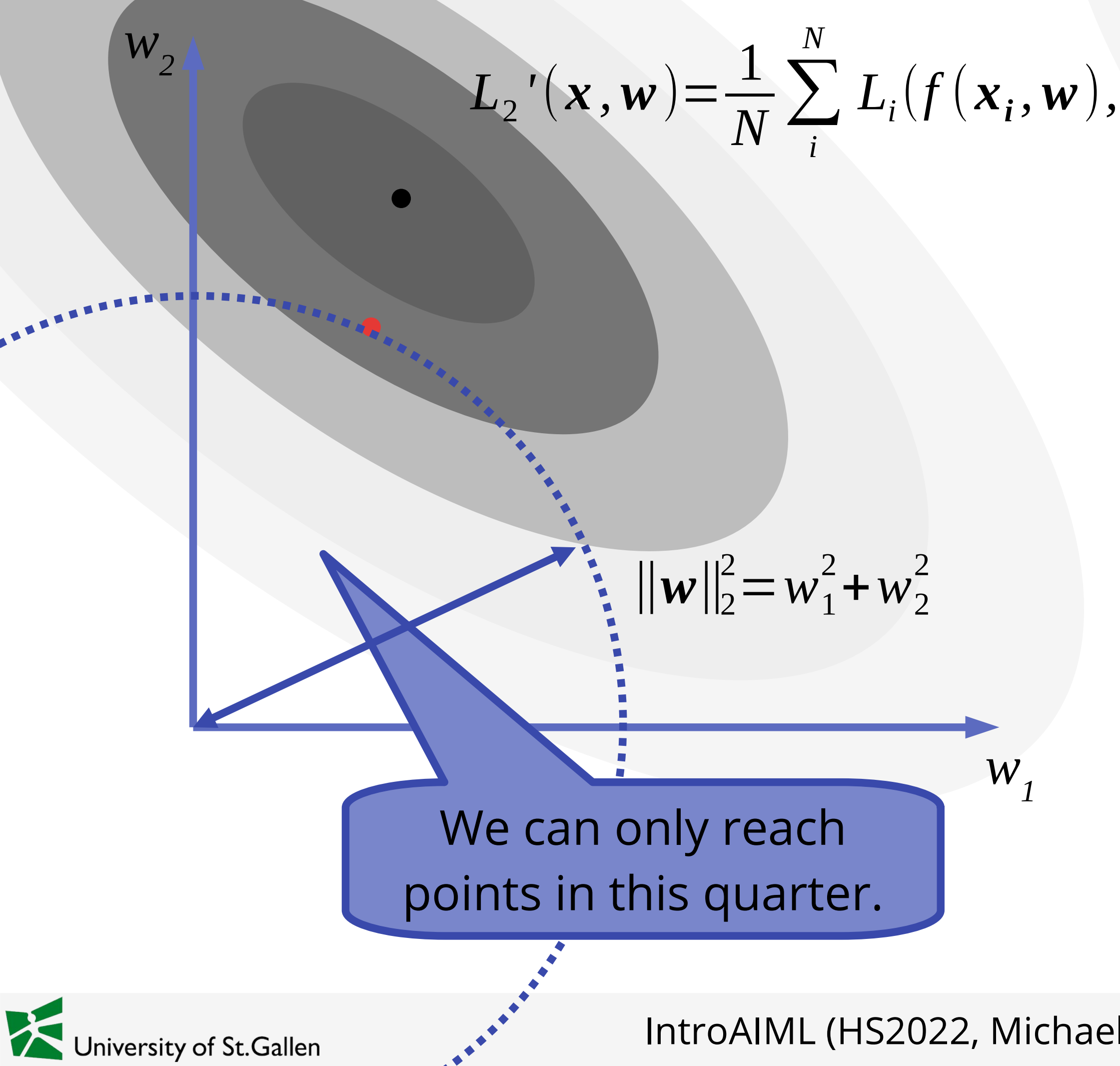

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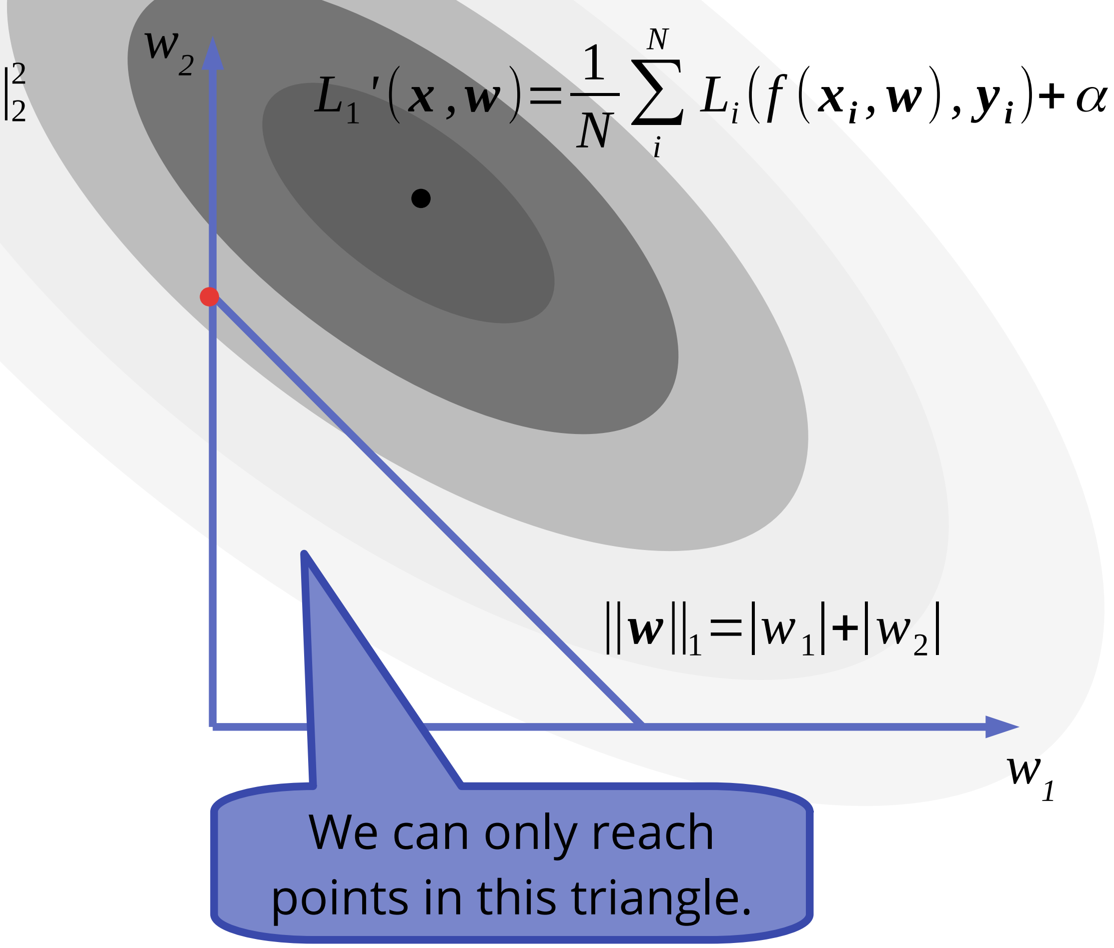

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Both regularization techniques are widely used in regression and classification tasks. They can be deployed in any machine learning model that minimizes a loss function.

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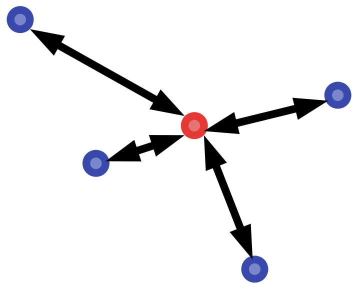
Nearest-Neighbor models



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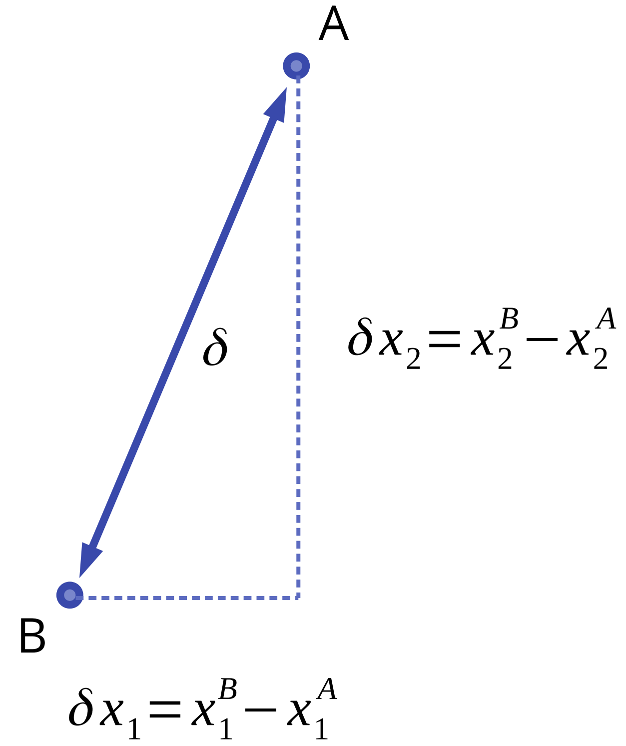

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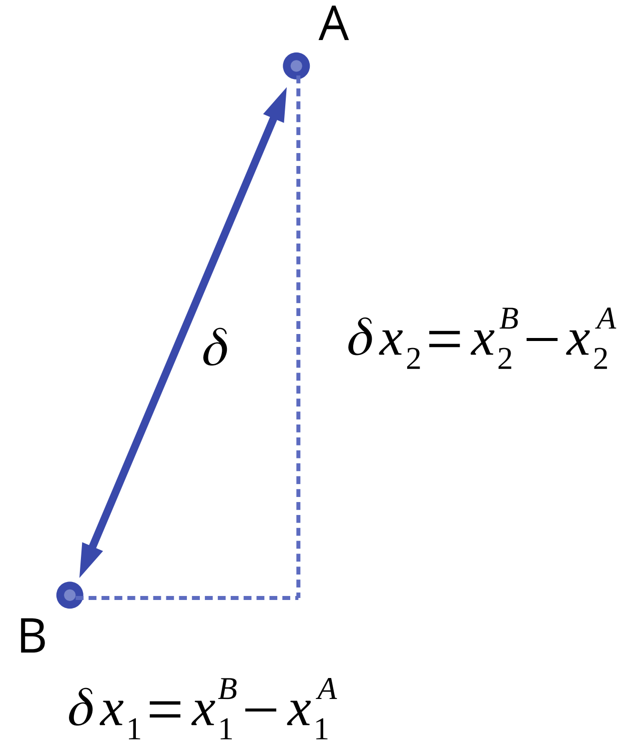

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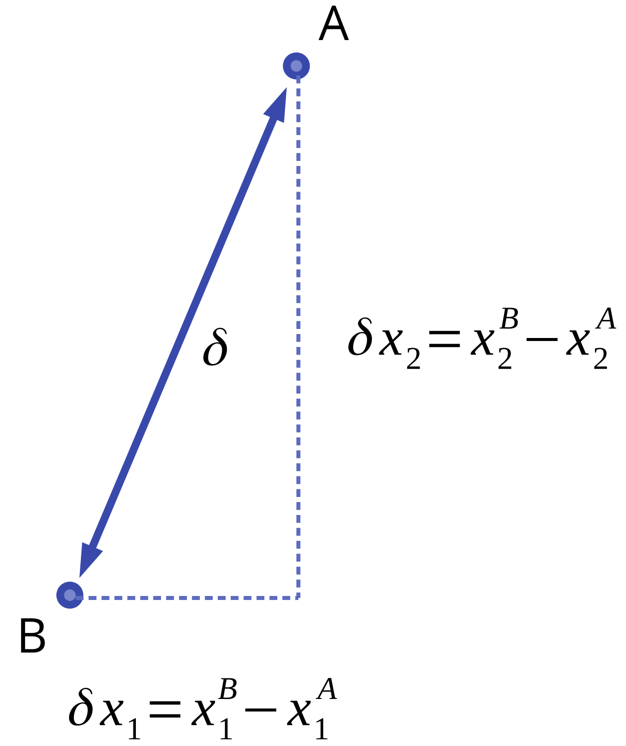
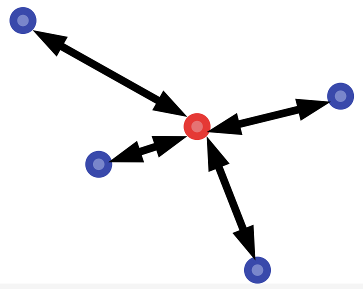


Nearest neighbor methods utilize distances between datapoints for **classification** and **regression** tasks.



k-nearest neighbor classification

k-nearest neighbor (knn) classifiers predict class affiliation of an unseen data point based on **majority voting** of its ***k* nearest neighbors** in a seen data set with ground-truth labels.

knn models are not trained in the general sense. Instead, the distance of each unseen data point from all seen data points is calculated.

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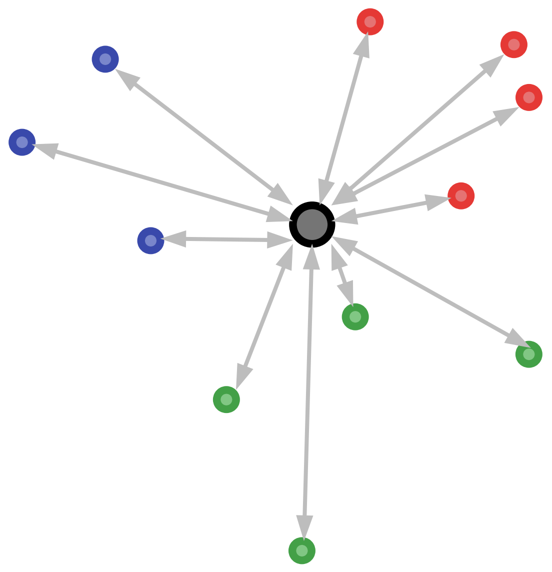

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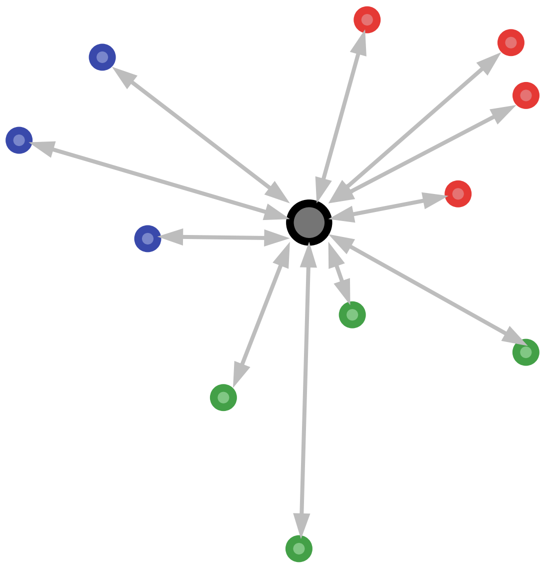

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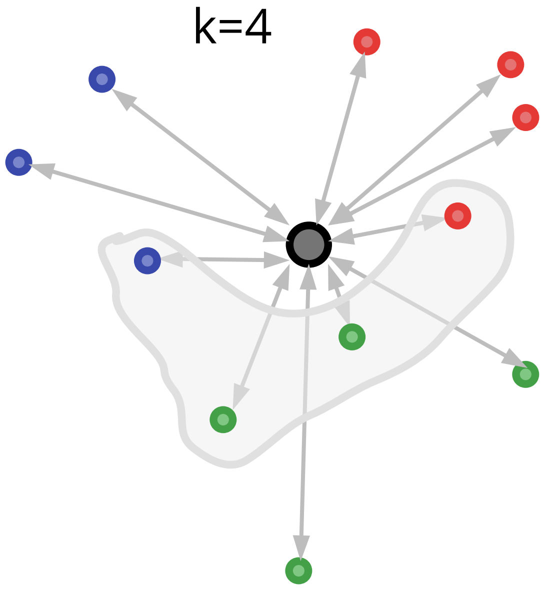

identify *k* nearest neighbors

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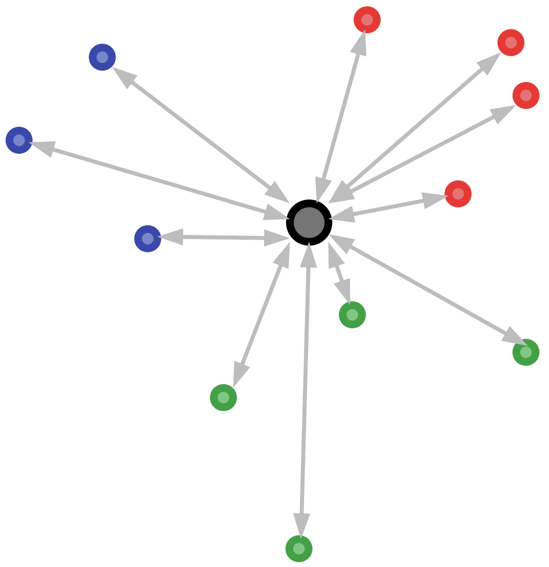

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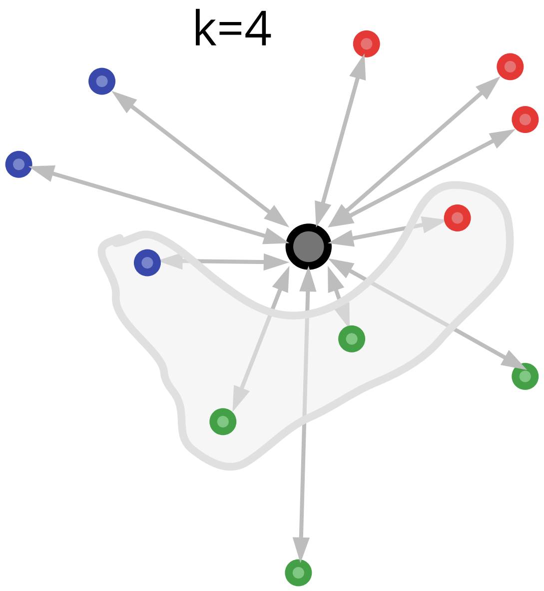

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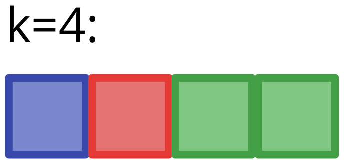

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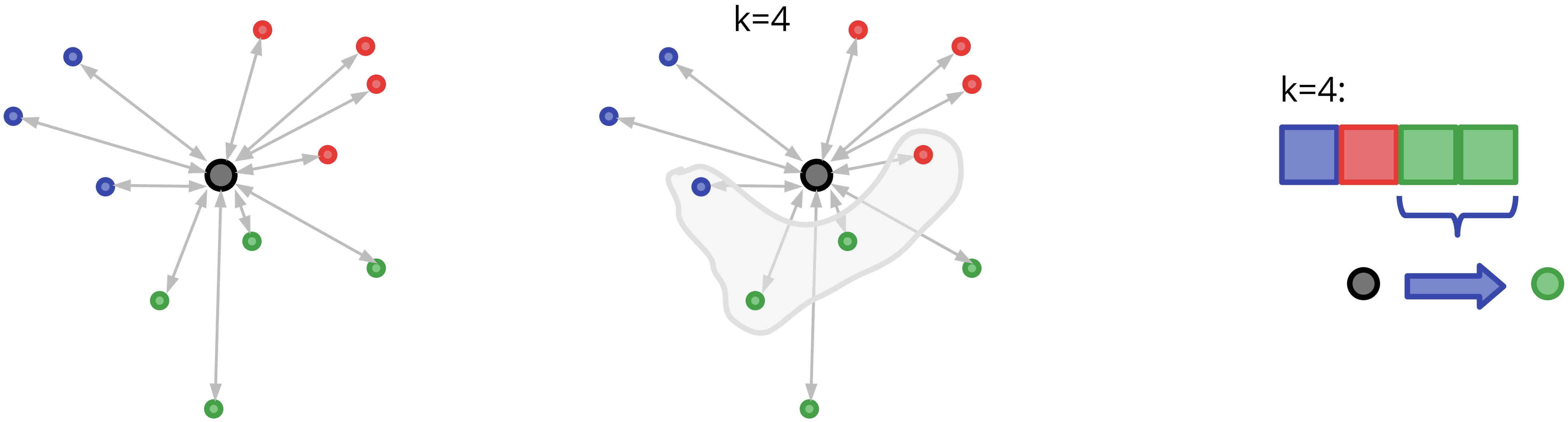
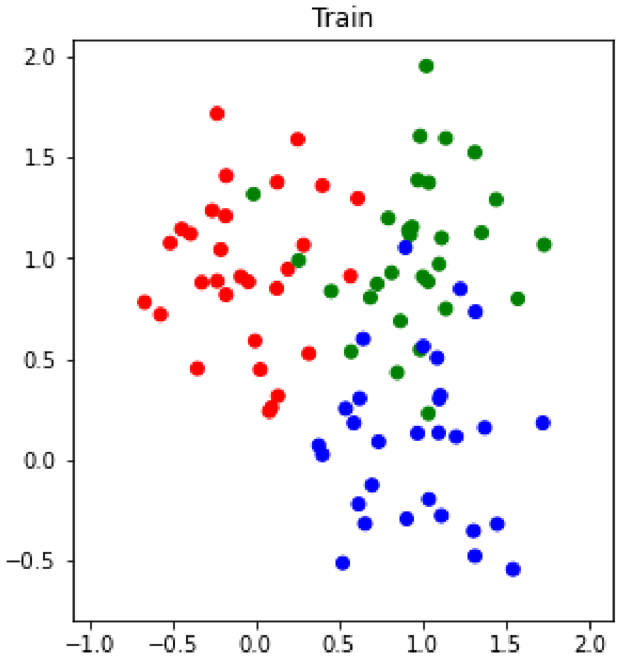
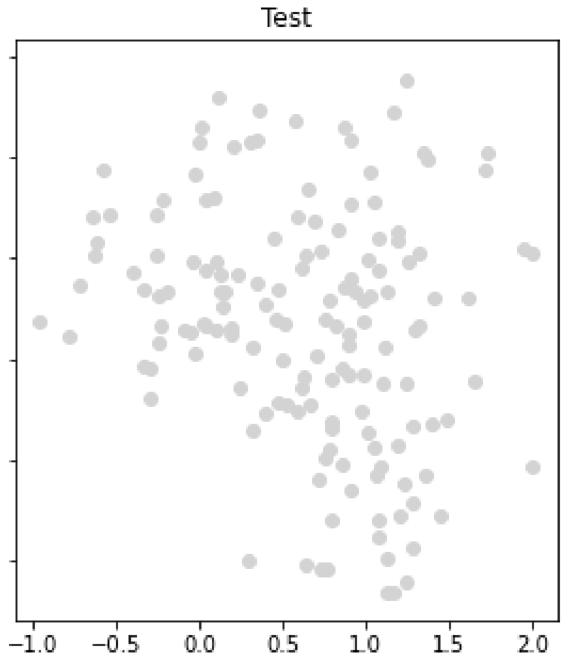


compute distances | identify *k* nearest neighbors | class assignment

k-nearest neighbor classification - Example

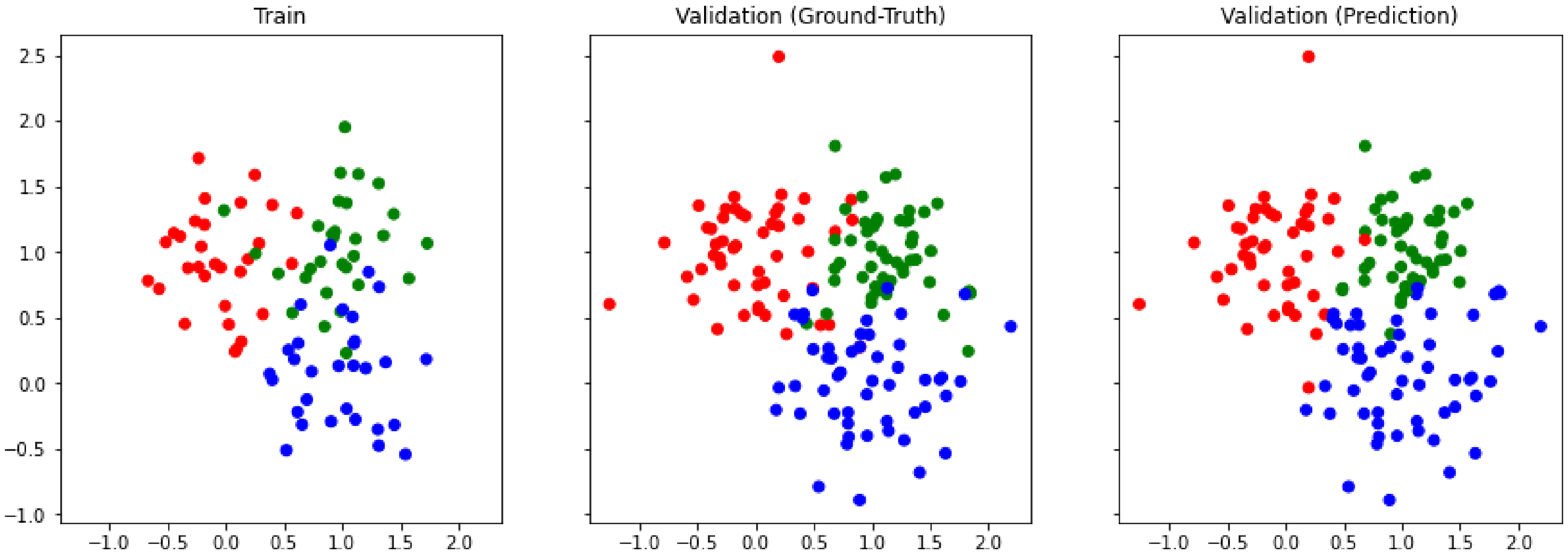




3 overlapping clusters

How well can knn classify our test data set?

k-nearest neighbor classification - Example



k=5: accuracy=0.867

Hyperparameter *k* has an impact on how well the model generalizes to unseen data: perform a **hyperparameter search**!

k-nearest neighbor classification - Example

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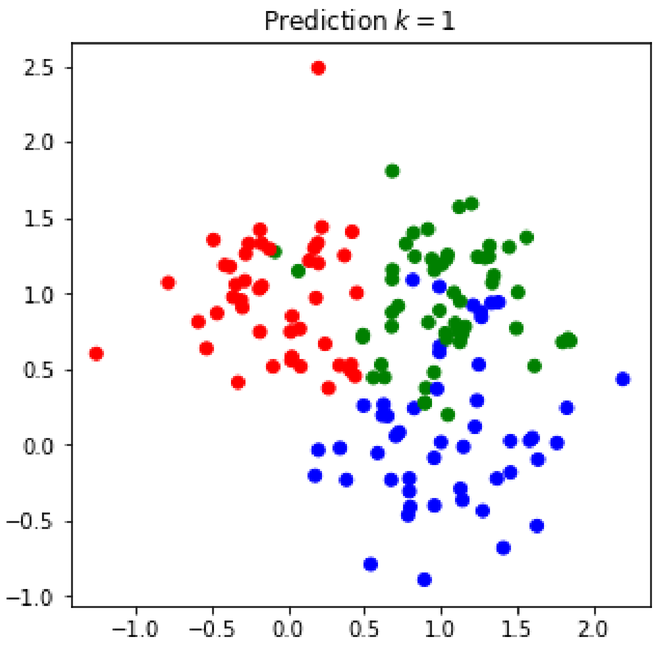
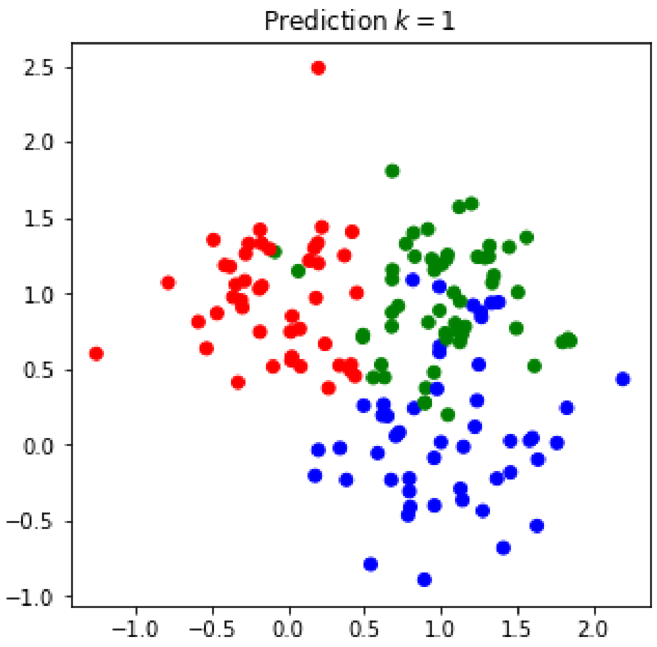


k=1

accuracy$_{\text{val}}$=0.800

k-nearest neighbor classification - Example



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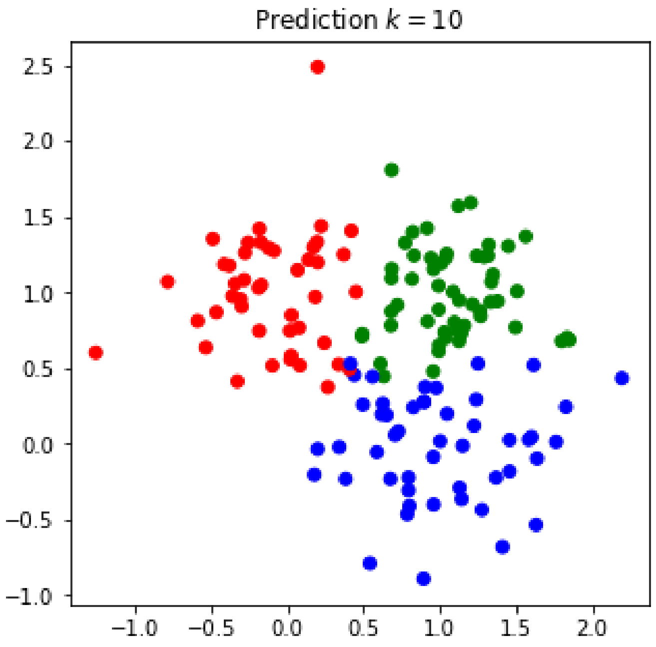
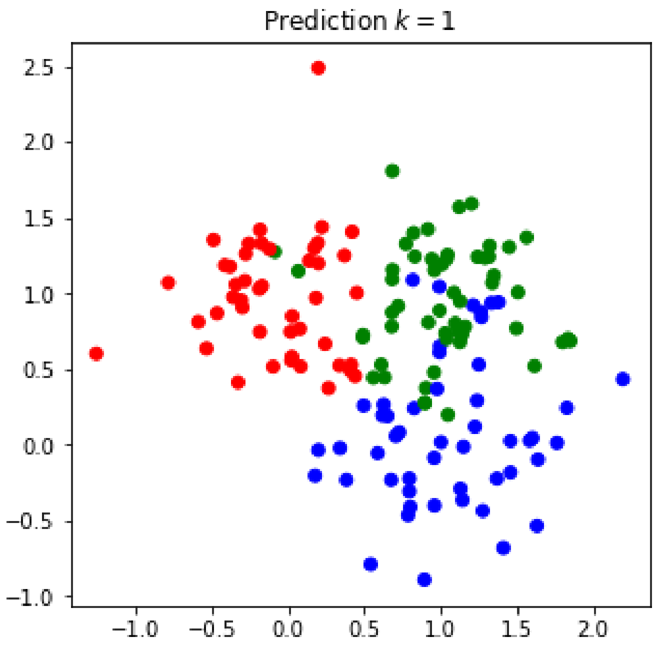


k=10
accuracy$_{val}$=0.893

k-nearest neighbor classification - Example



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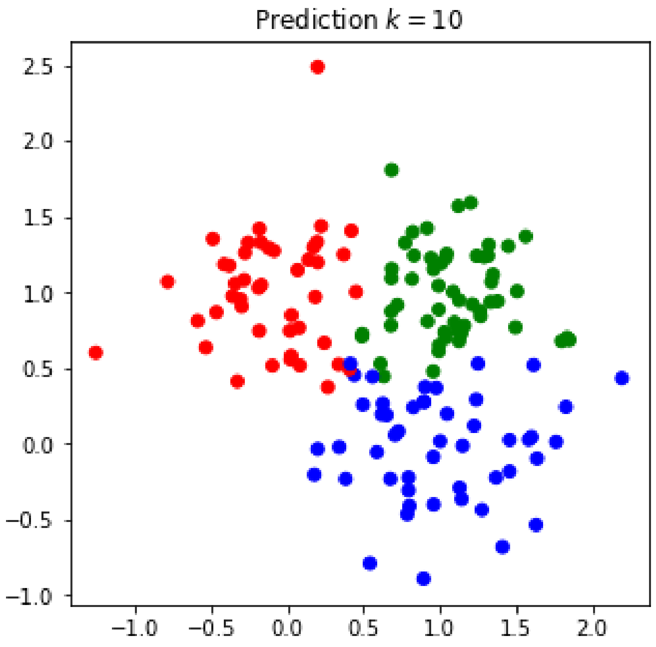

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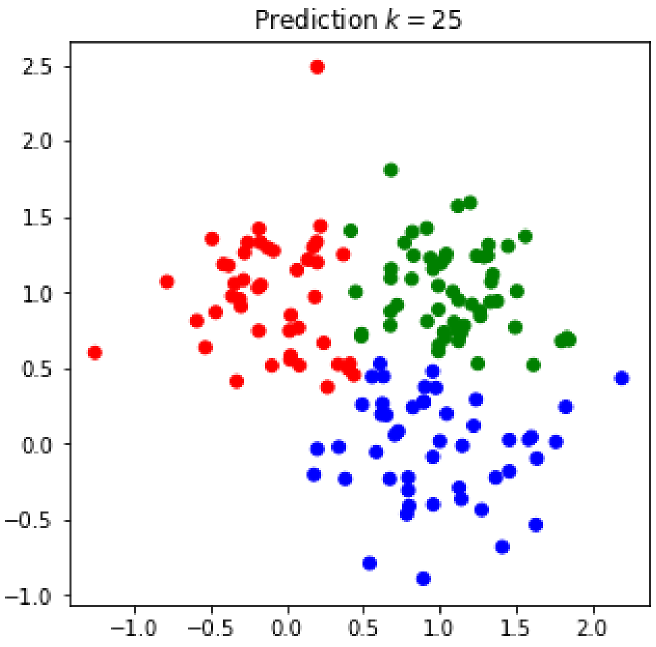
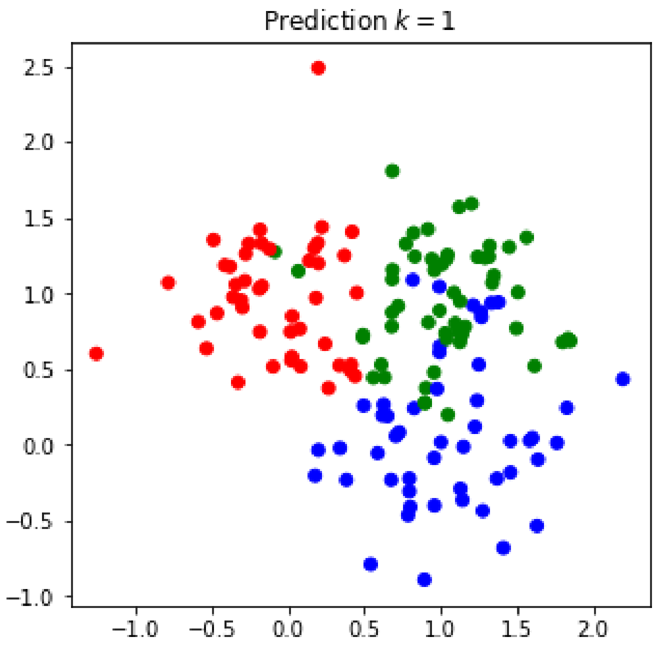


k=25
accuracy$_{val}$=0.873

k-nearest neighbor classification - Example



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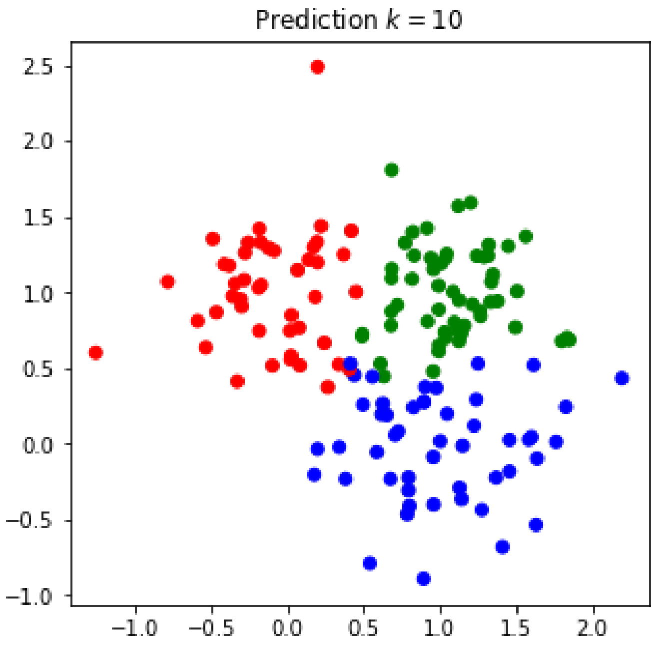
Overfitting!

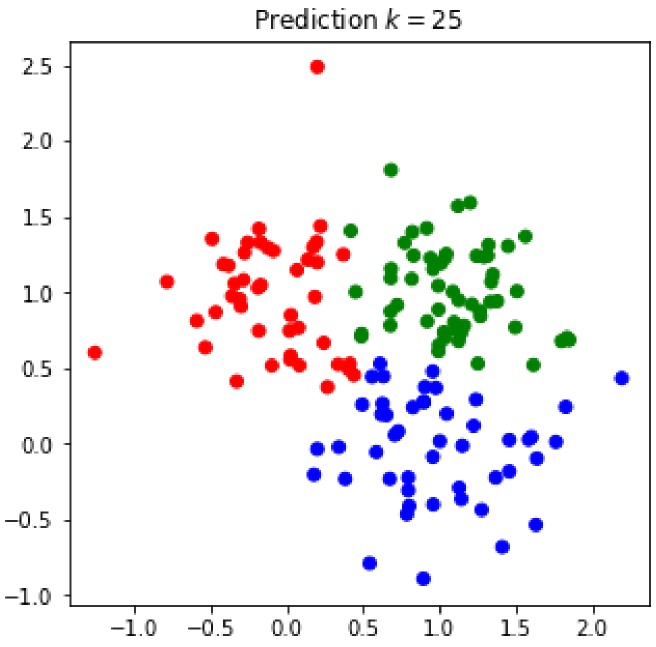


k=10

accuracy$_{val}$=0.893

accuracy$_{test}$=0.880

Best performance



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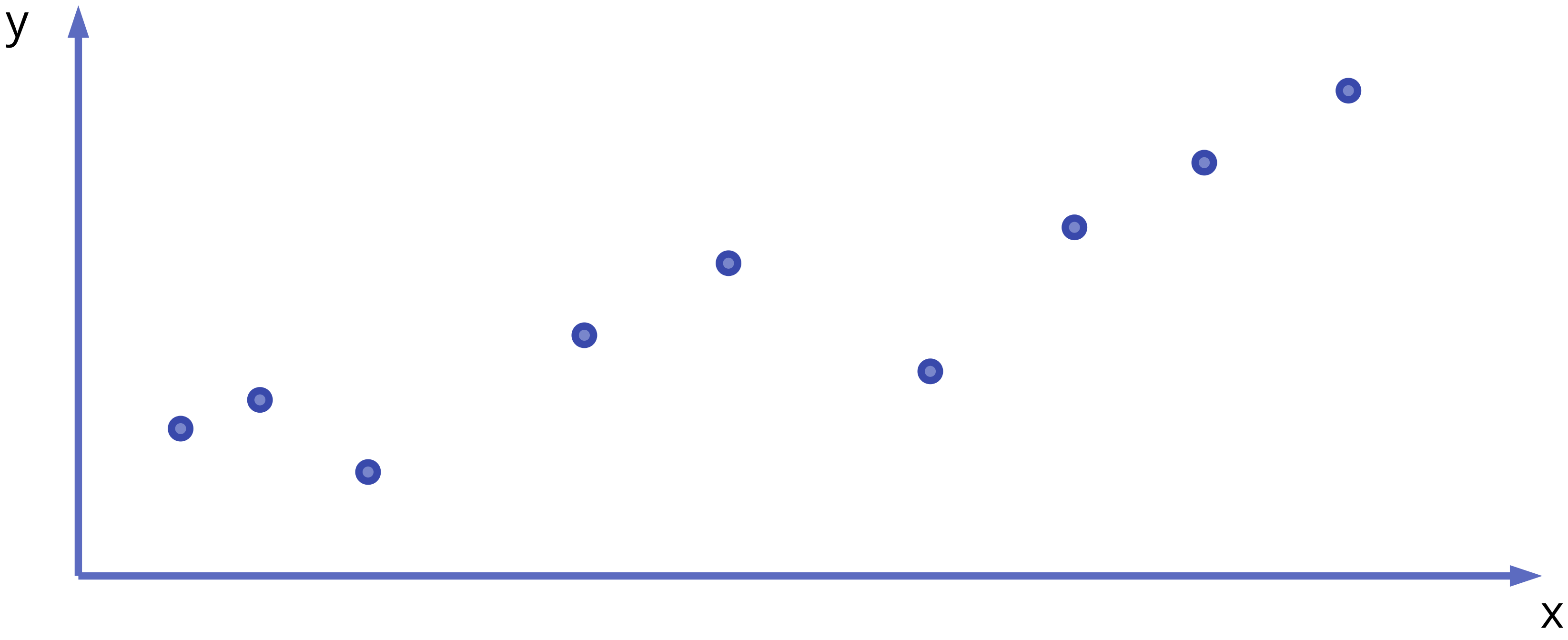
Underfitting!

k-nearest neighbor regression

Nearest neighbor methods can also be implemented as regressors that are able to **interpolate** between and **smoothen** available data.



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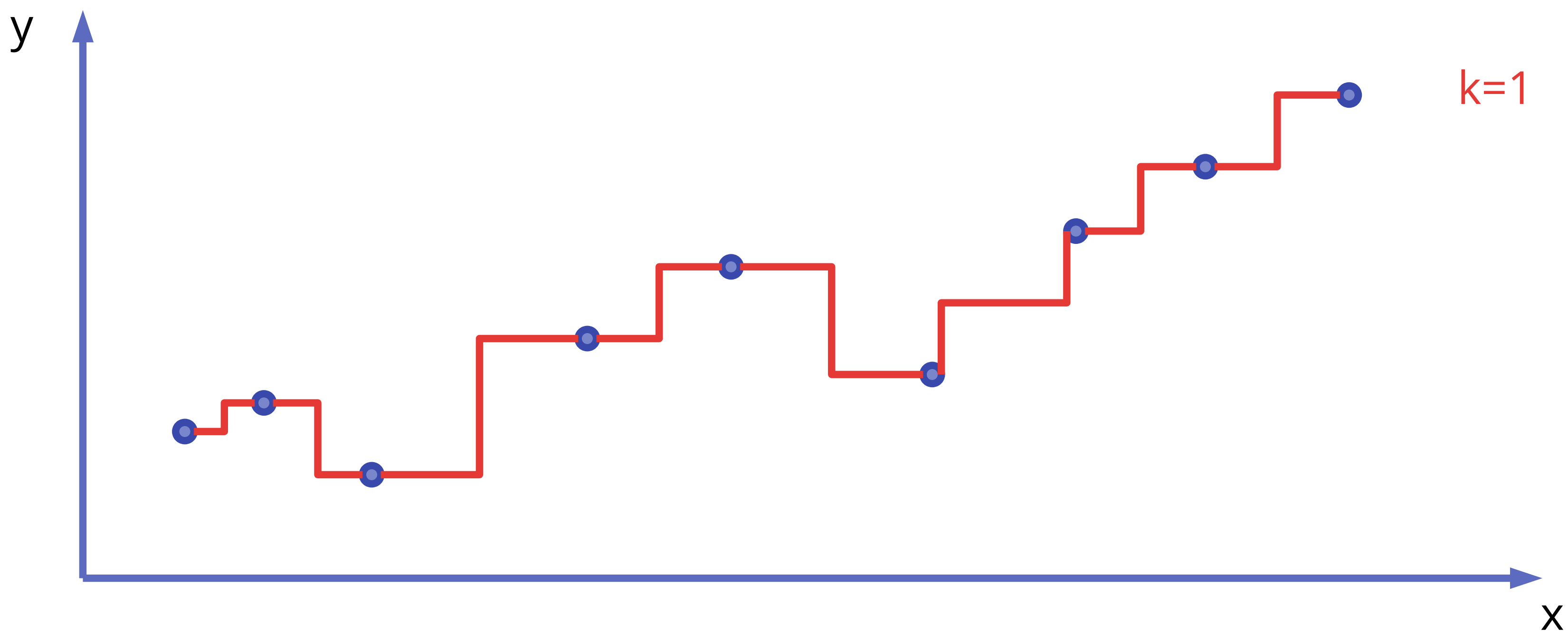

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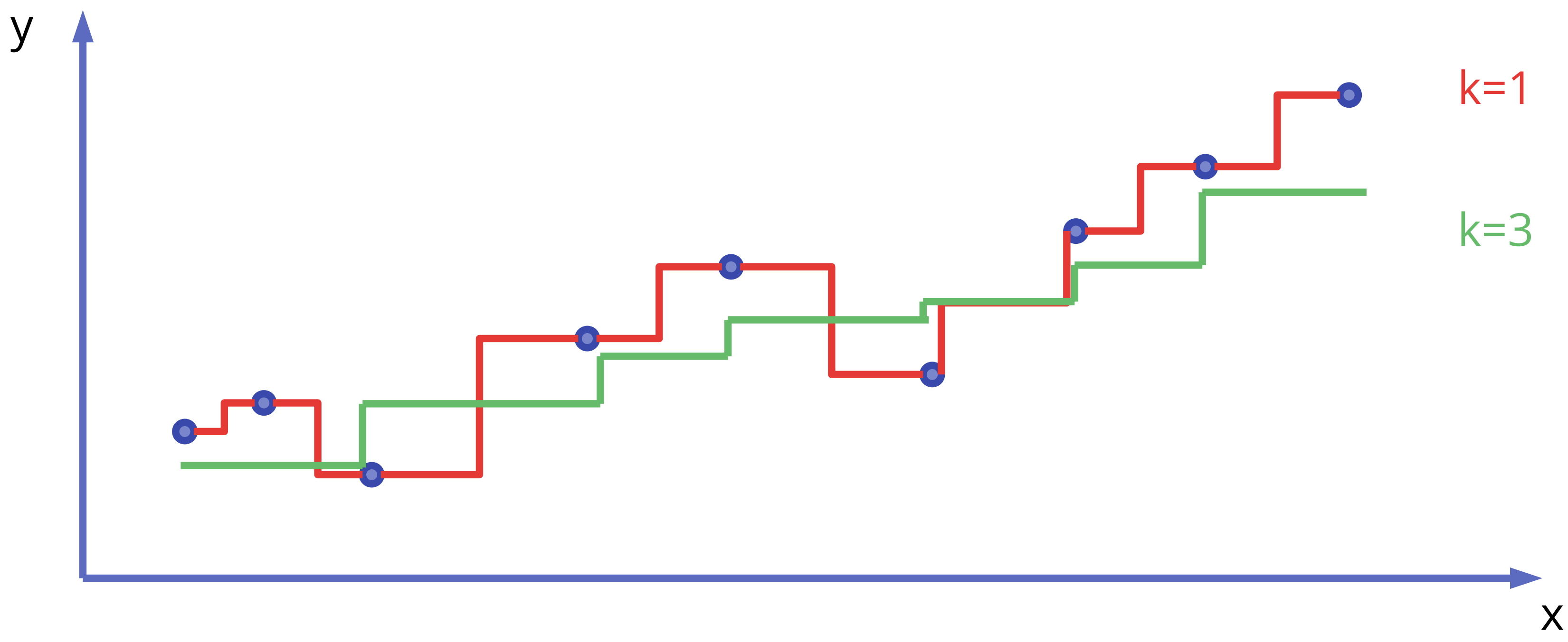

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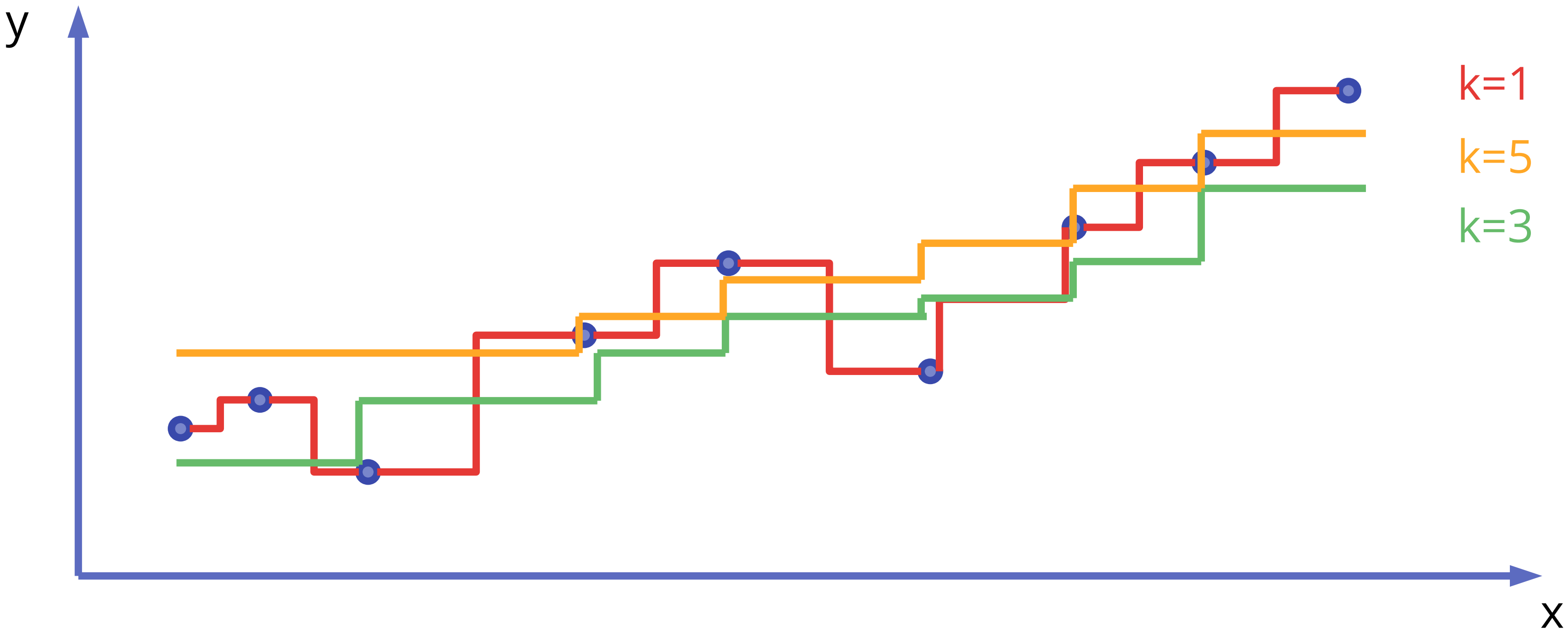

Regularizing nearest neighbor methods

Regularizing nearest neighbor methods is simply done through varying its hyperparameter, k.

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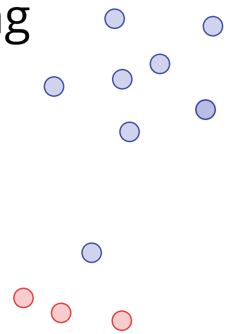

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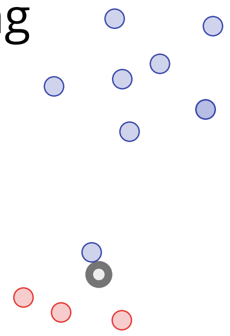

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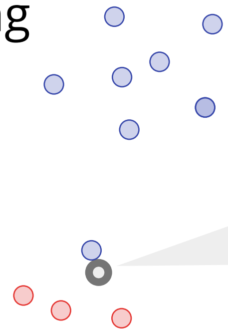

k=1: blue
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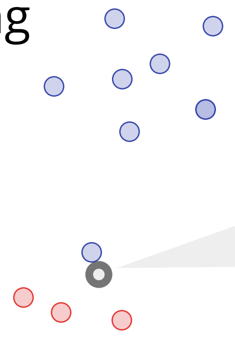

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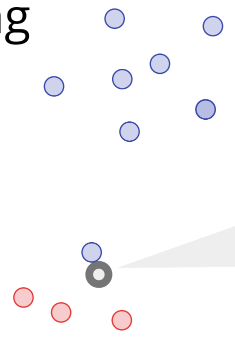

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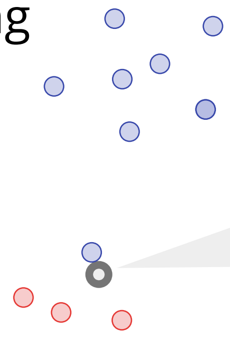

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A high k may miss local details.

k-nearest neighbor classification – pros and cons

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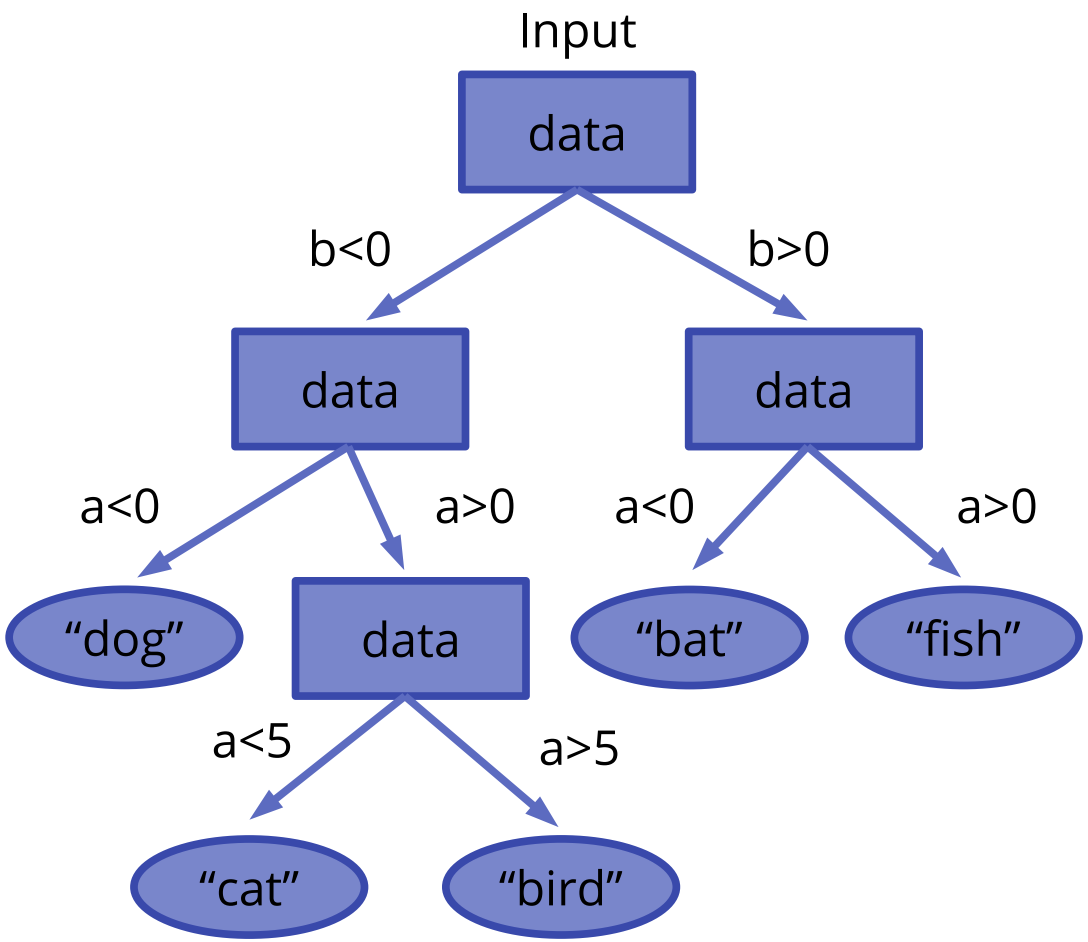
Number of data points should grow exponentially with data dimensionality.

If parameter space is insufficiently sampled, the model does not have enough data points for training properly.

Tree-based models (a high-level introduction)



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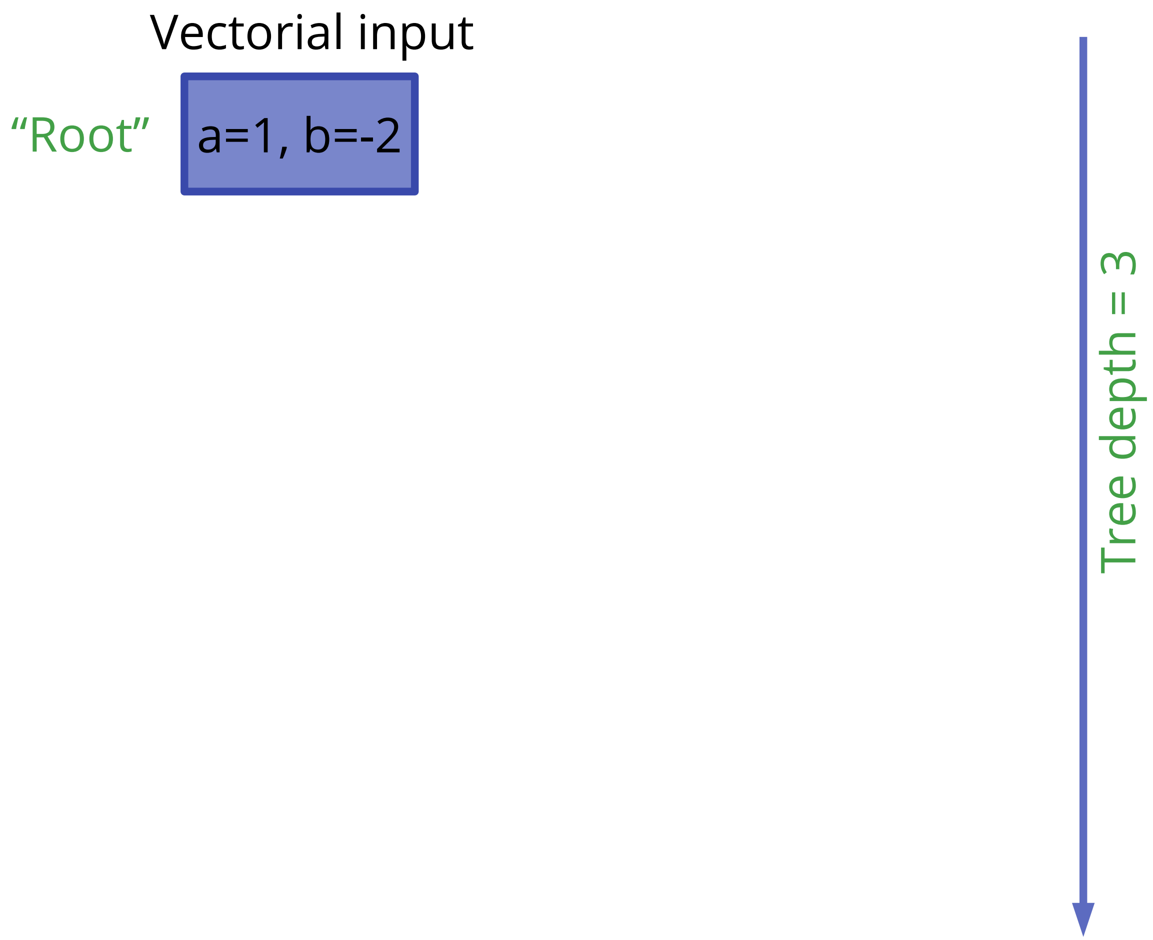

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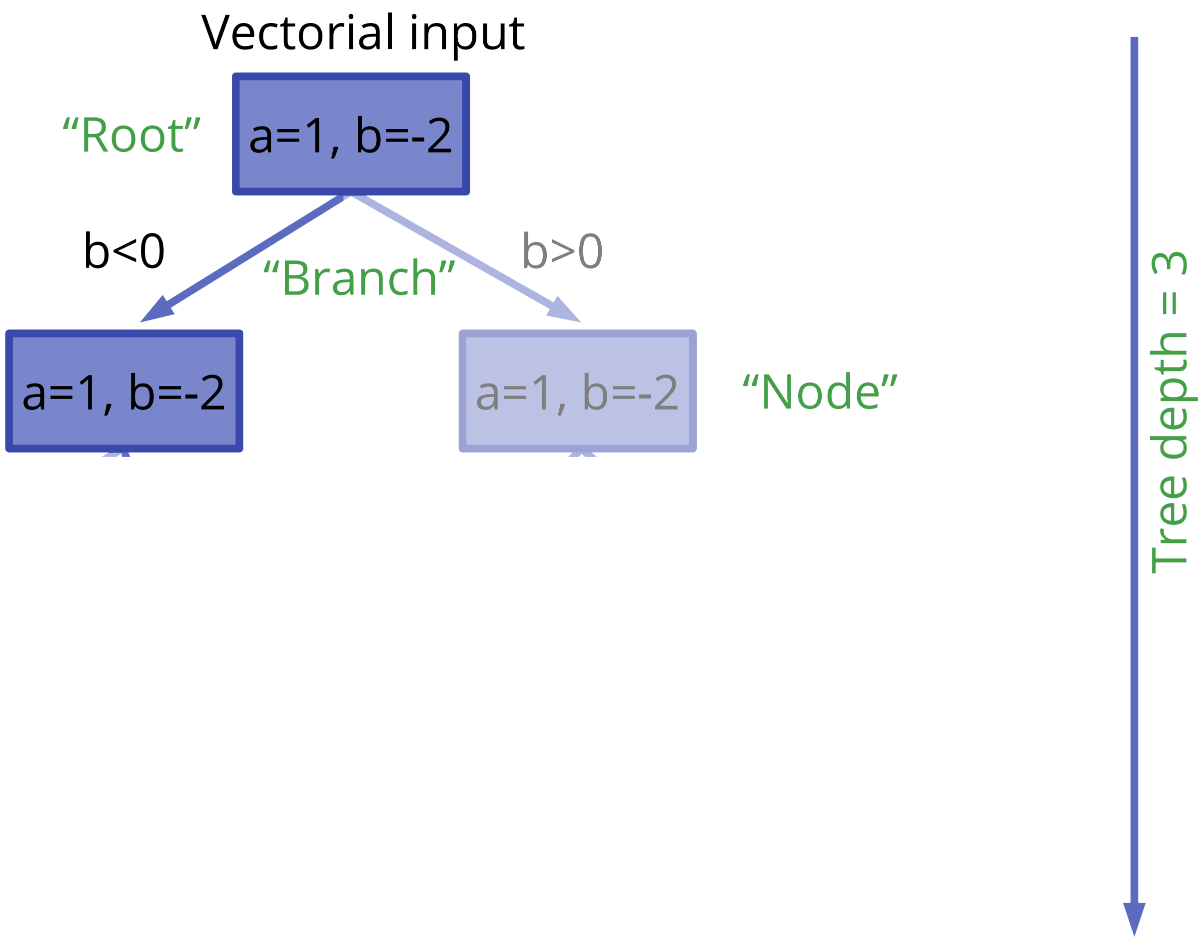

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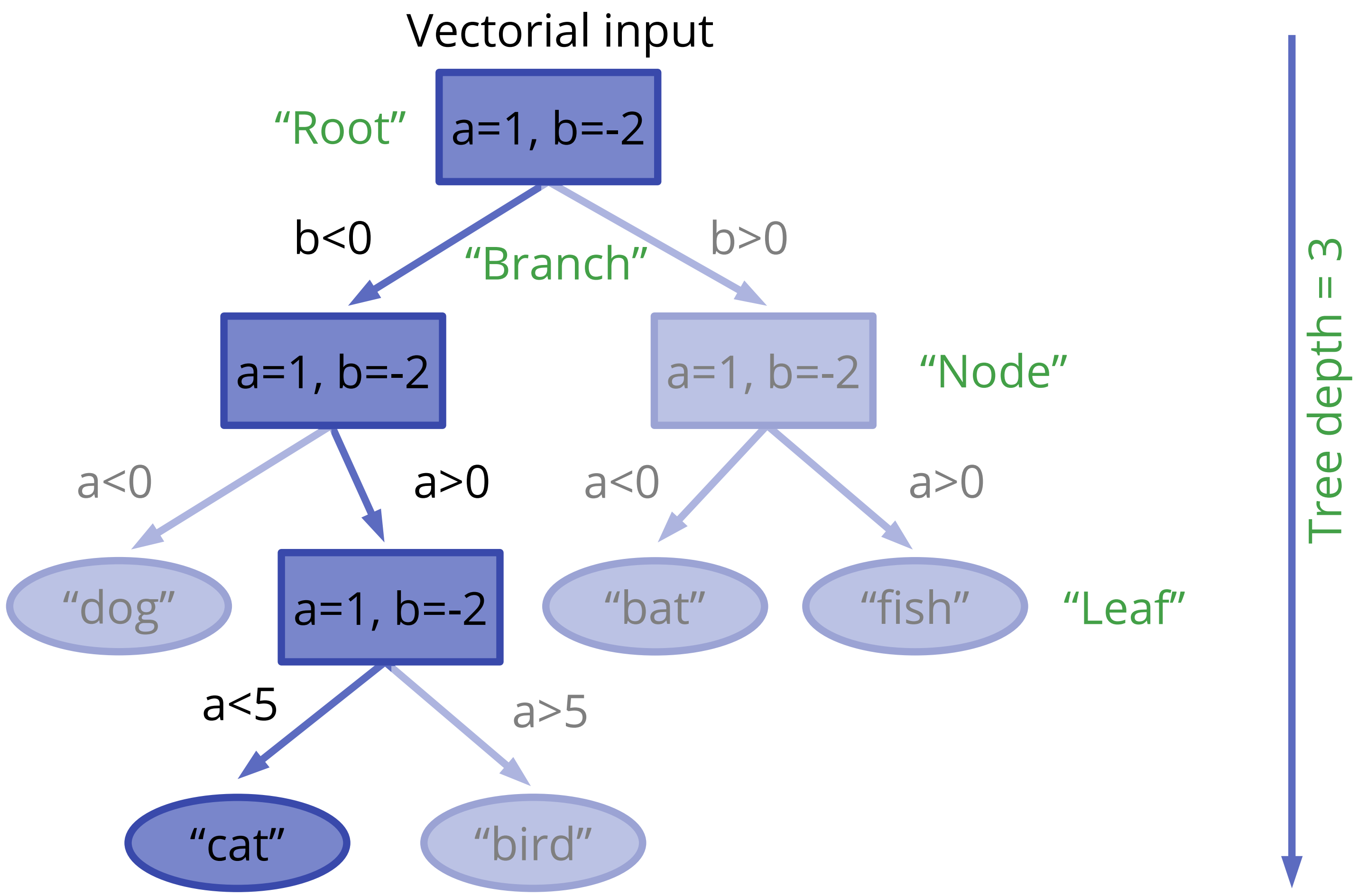

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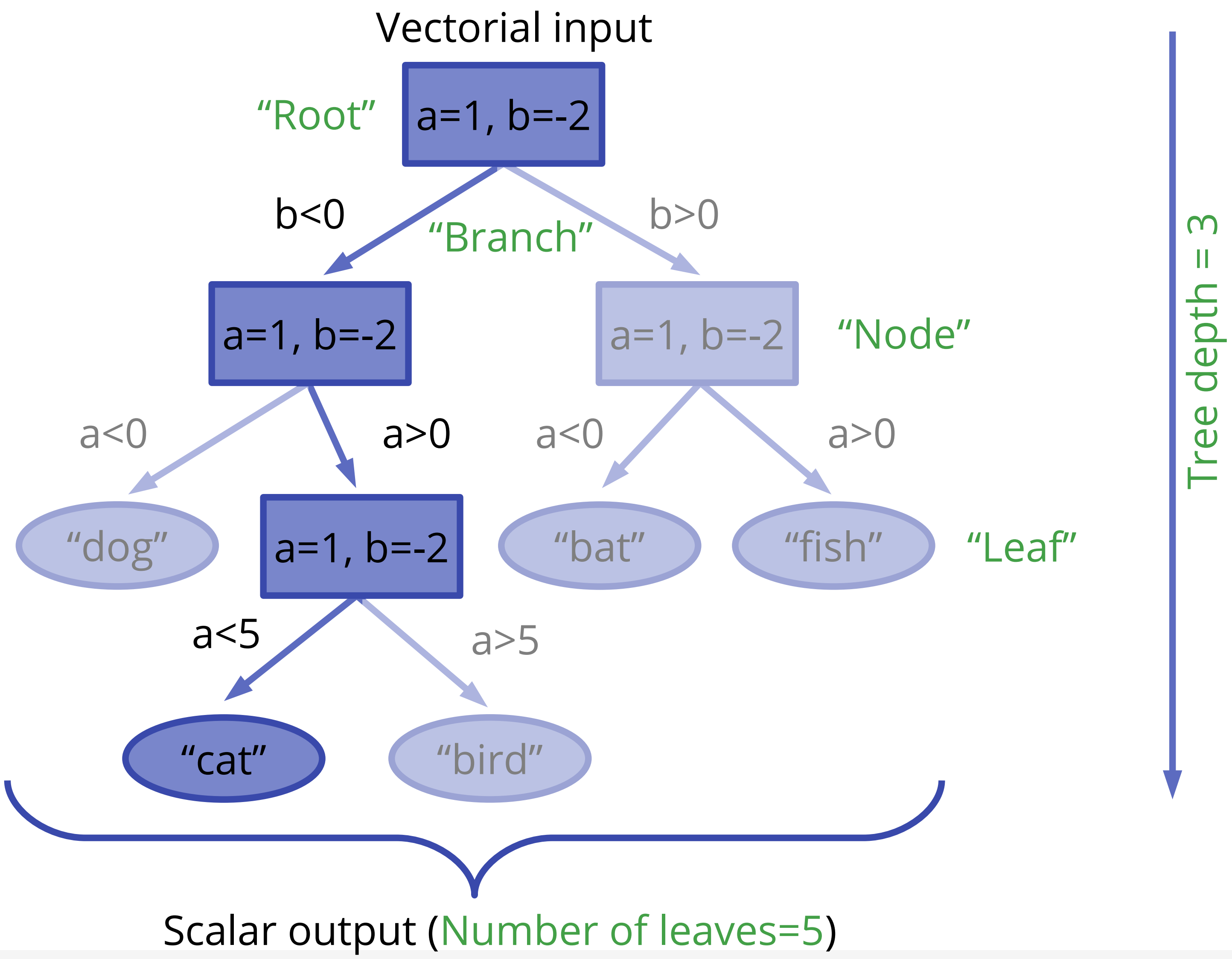

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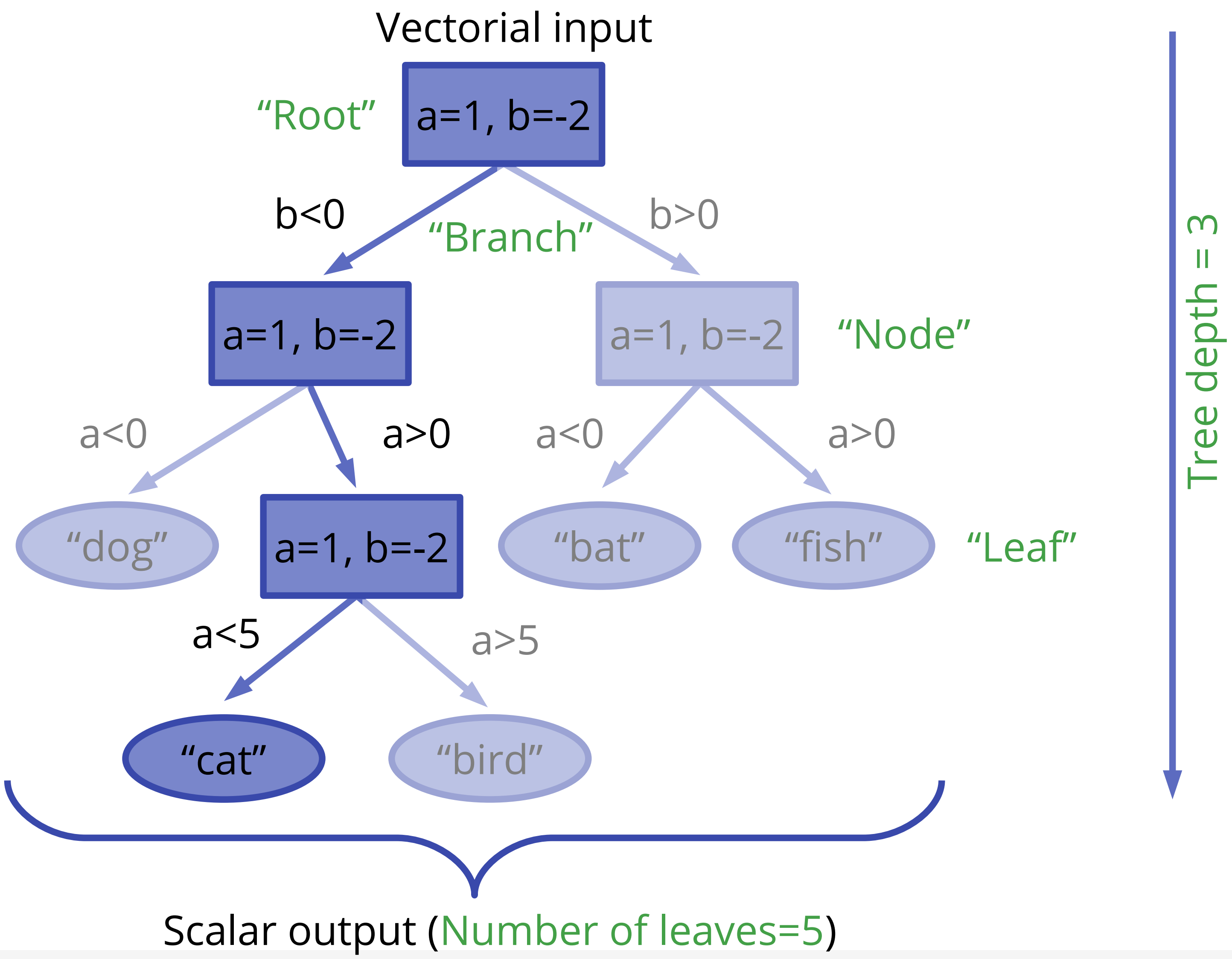
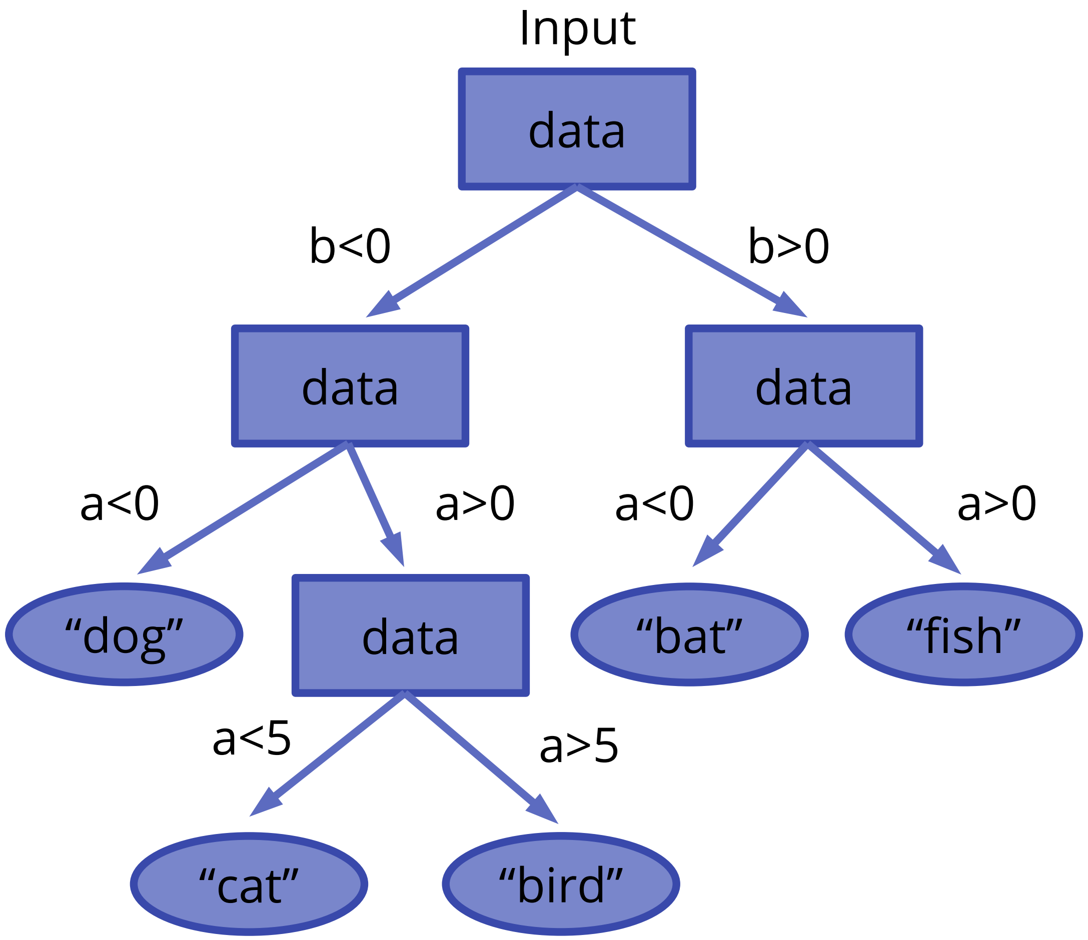
How can the rules stored in the nodes be learned?



Decision tree learning



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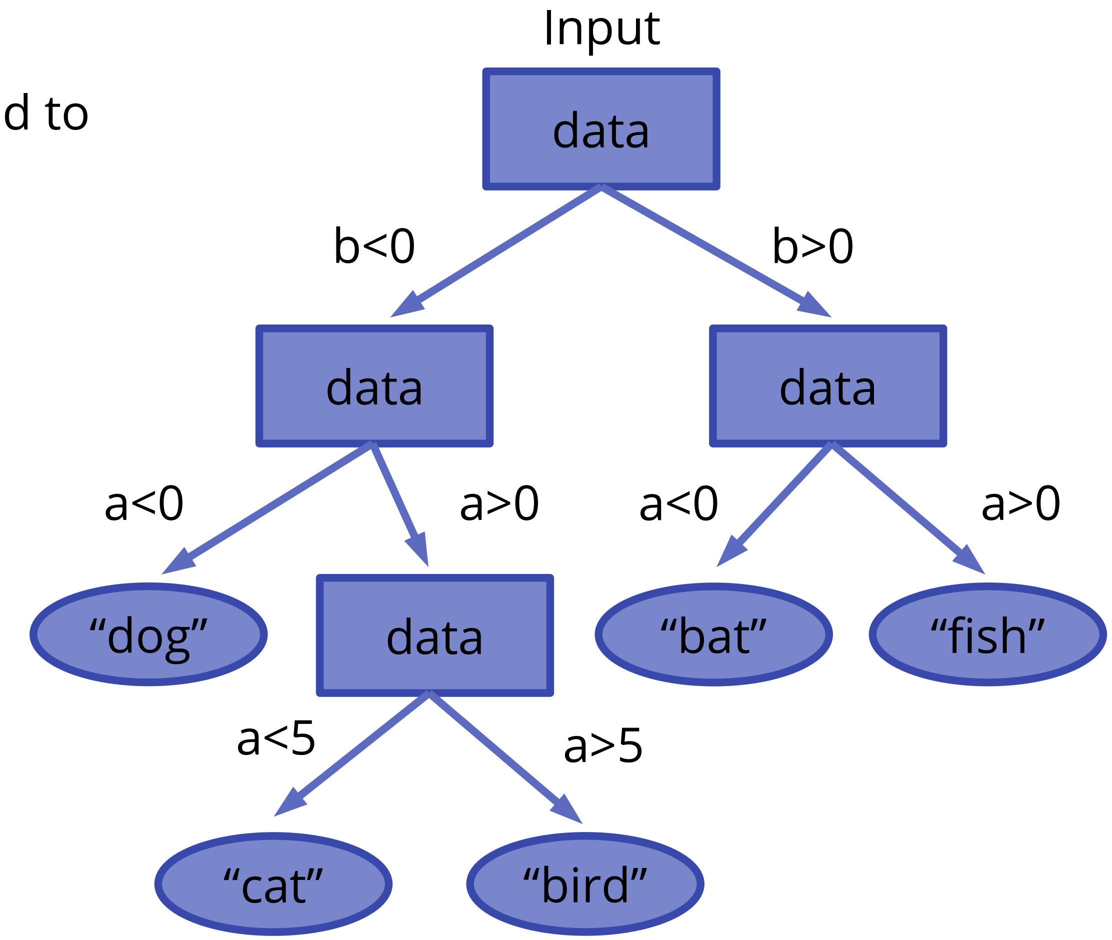

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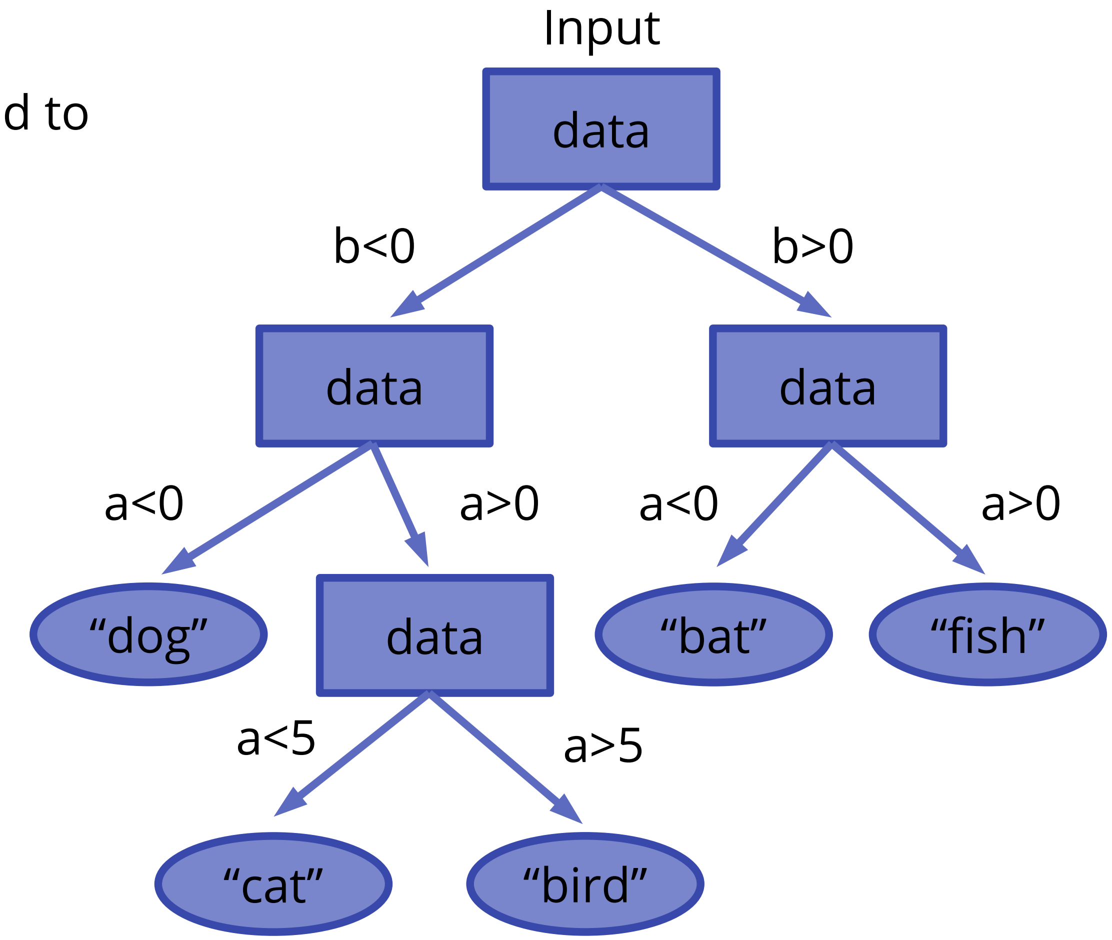

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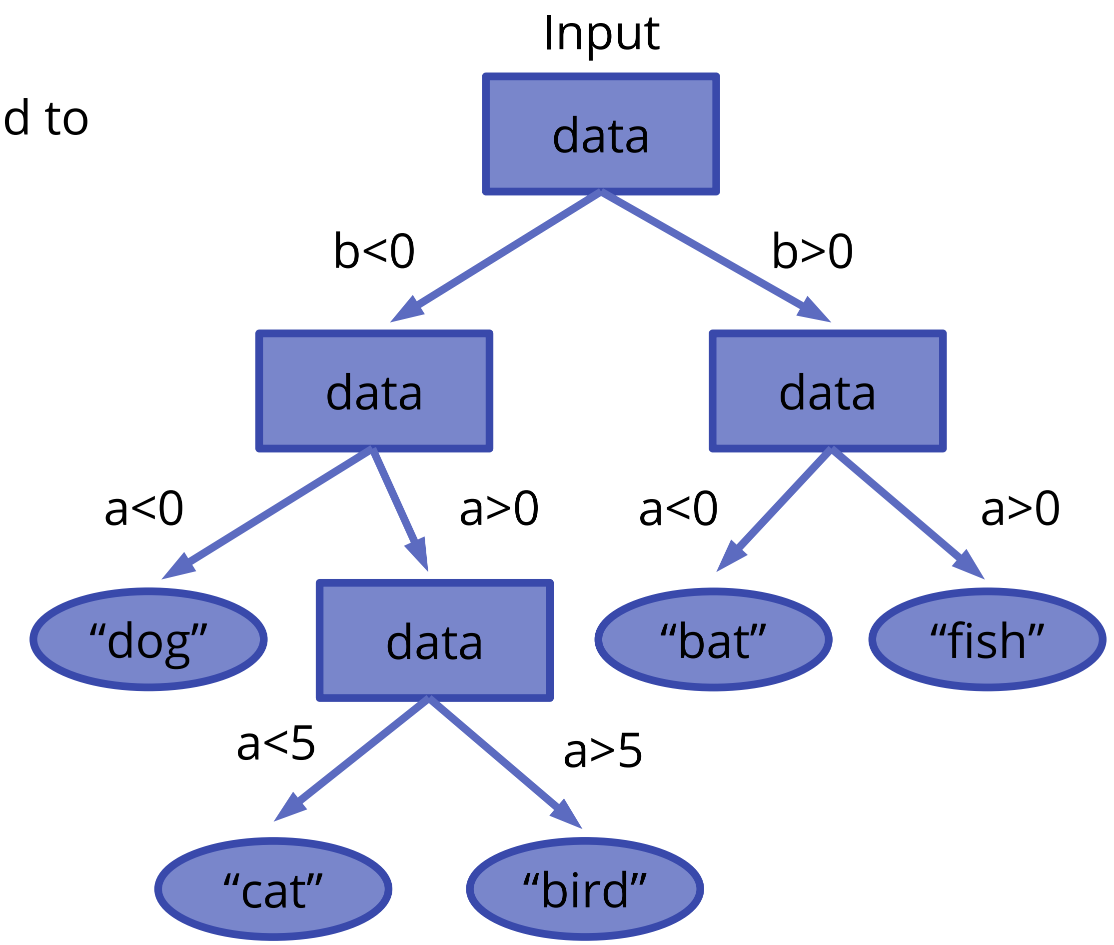

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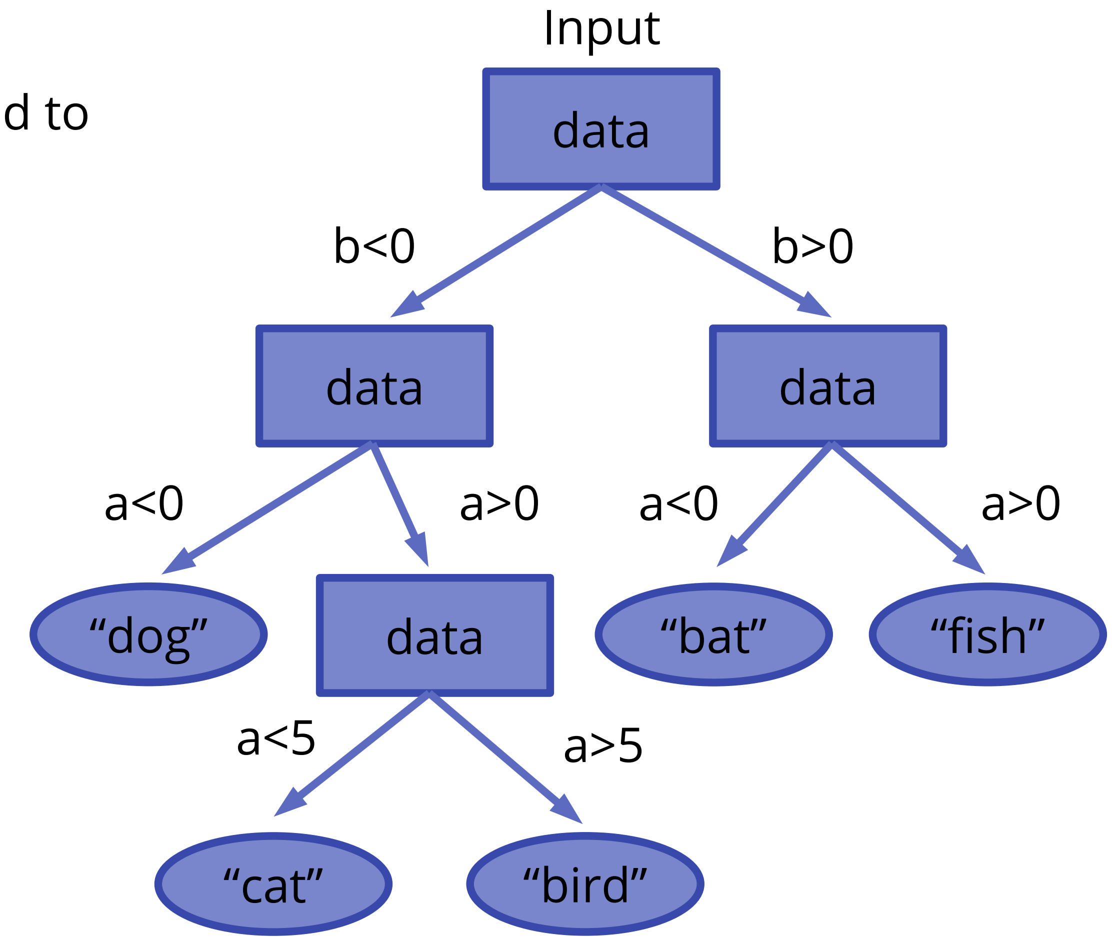

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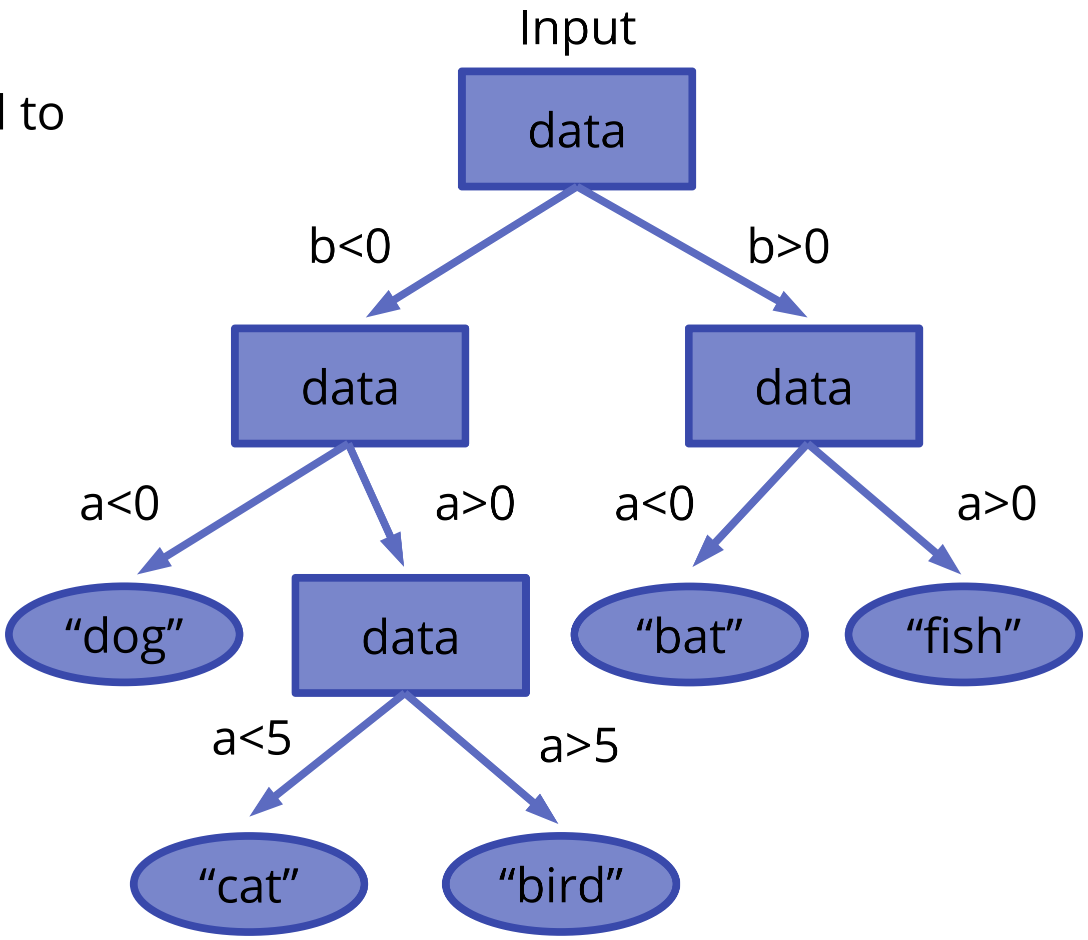

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But what is the “most important feature”?

Generally, it means that feature that makes the most difference to the classification of a single sample.

There different implementation of this definition, e.g., utilizing **information entropy** or other useful measures.

Random forests - decision trees as “weak learners”

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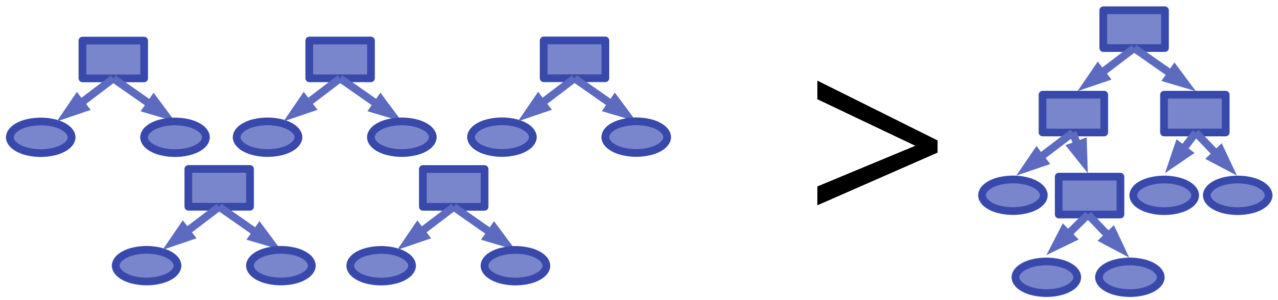

Gradient-boosted tree-based models

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The term **gradient-boosting** refers to the fact that new base learners (individual decision trees) are fitted to the model's pseudo-residuals, based on the gradient of the loss of the ensemble:

$$f(\mathbf{x}) = \sum_{m}^{M} \beta_m h(\mathbf{x}, \theta_m)$$

Ensemble model with learning rate β_m, base learners $h(\mathbf{x}, \theta_m)$ with parameters θ_m.

$$\boldsymbol{r}_{\boldsymbol{m}}^{\boldsymbol{i}} = -\left[\frac{\partial L(y^i, f(x^i))}{\partial f(x^i)}\right]_{f=f_{m-1}}$$

Pseudo-residuals to which the next base learner will be fitted; by default, the loss of the updated ensemble will be less or equal to the loss of the current ensemble.

Gradient-boosted tree-based models

Gradient-boosted models are very successful in regression and classification tasks and still represent state-of-the-art in traditional ML.

If you have a classification or regression problem, it is always worth trying out gradient-boosted methods.

Common implementations:

- XGBoost
- LightGBM

Tree-based models – pros and cons

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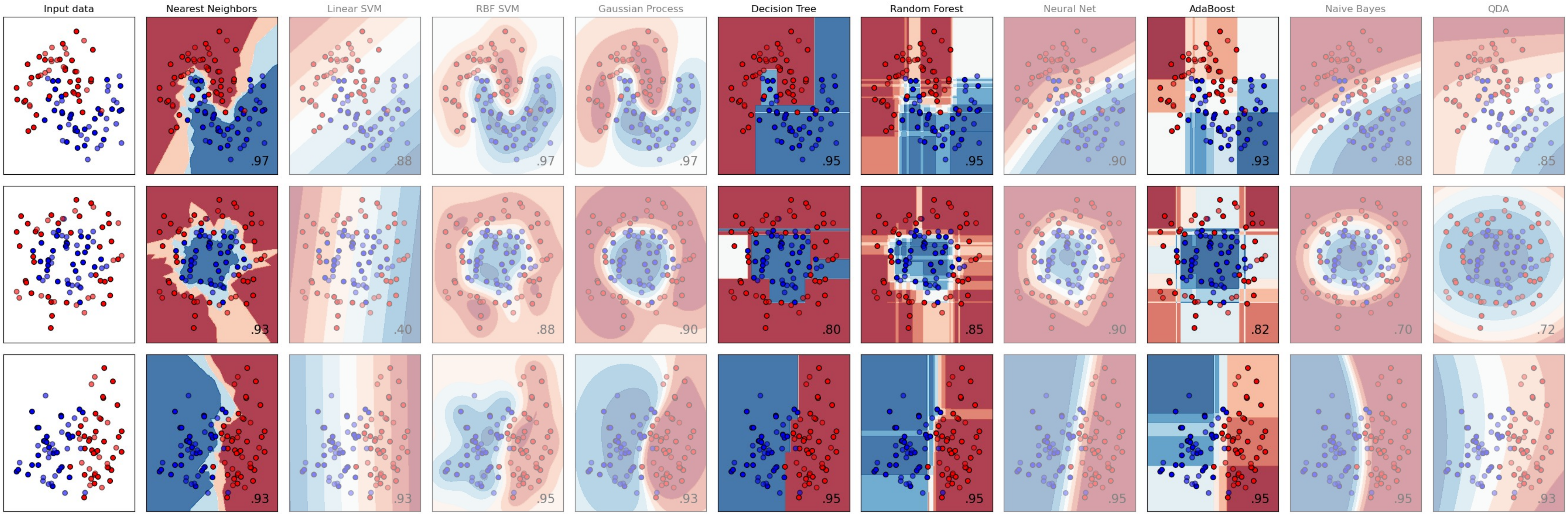
Cons:

- Decision boundaries and regression predictions may be discrete instead of continuous (see next slide)

Supervised learning - summary



(Similar to XGBoost)

Scikit-learn classifier comparison

That’s all folks!

Today's lecture

Linear models

Nearest Neighbor models

Tree-based models

Today's lecture

Supervised learning methods

Linear models

Nearest Neighbor models

Tree-based models

Today's lab course:
Supervised Learning!

Next lecture (6 Oct)

Search (Guest lecture by Damian Borth)

Search problems

Breadth-first search

Depth-first search

Greedy search

A* search