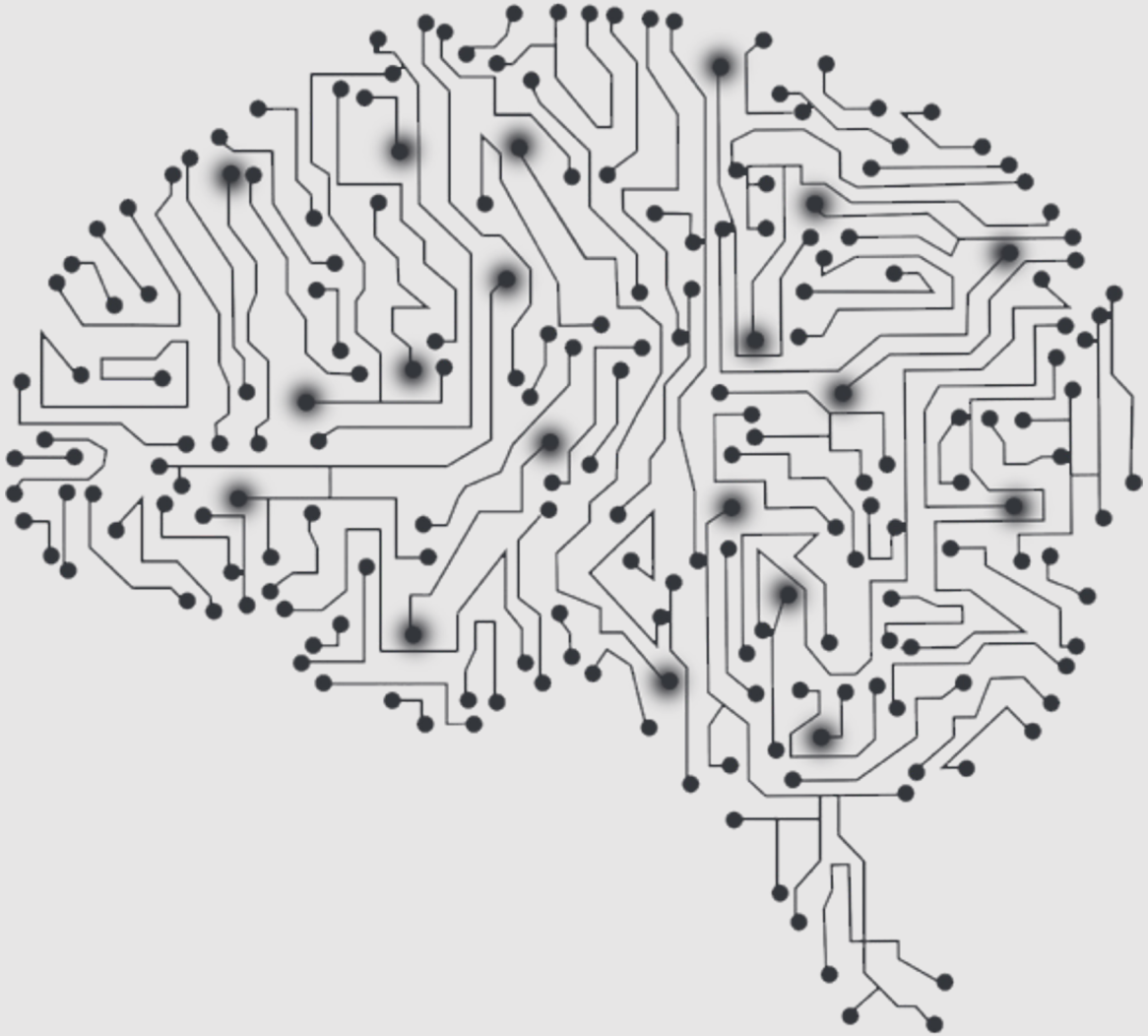
LECTURE 1

INTRODUCTION TO DEEP LEARNING



Tsvigun Akim

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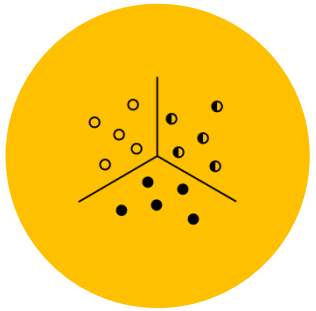
Lecture Plan

1. Revise general ML notions
2. Gradient Descent
3. Overfitting
4. Gradient Descent Extensions
5. **Neural Networks!**
    1. How to build a more expressive model?
    2. Nonlinearity
    3. Backpropagation and Chain Rule

Machine Learning Tasks

REGRESSION

CLASSIFICATION



CLUSTERIZATION

DIMENSIONALITY REDUCTION

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Machine Learning Areas

TABULAR DATA ANALYSIS

UNSUPERVISED LEARNING

TIME SERIES ANALYSIS

NATURAL LANGUAGE PROCESSING

COMPUTER VISION

AUTOMATIC SPEECH RECOGNITION

RECOMMENDER SYSTEMS

REINFORCEMENT LEARNING

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Supervised learning example

$a(x)$ → 13

ML pipeline attributes

- Model parameters (e.g. weights, predicates etc.)
- Forward pass (rule / formulae to make the predictions)
- Hyperparameters
- Loss function
- Optimization Algorithm
- Quality Metrics

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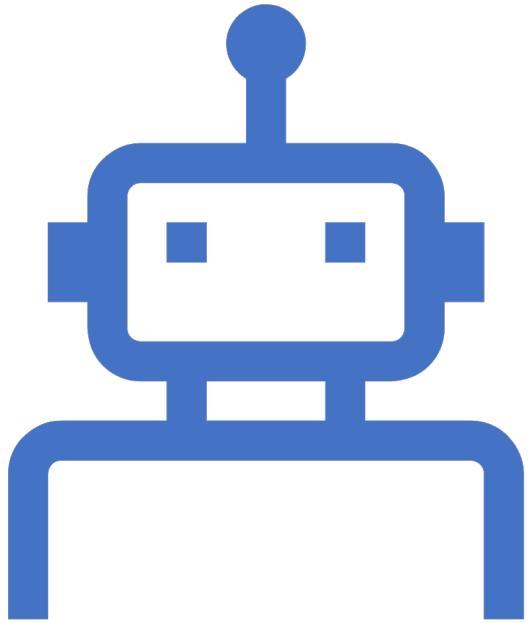
Model families

- Linear (linear / logistic regressions, SVM)
- Tree-based algorithms (decision trees, random forest, gradient boosting)
- Nearest Neighbors Methods (kNN)
- **Neural Networks**



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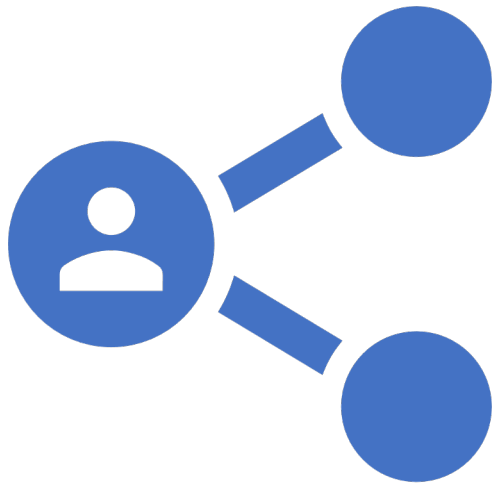
Features types

- Binary (0/1)
- Numerical (3.14)
- Categorical (’Liverpool’/ ’Chelsea’)
- Ordinal (sorted categorical: e.g. day of the week)



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Supervised learning

x_i — example

y_i — target value

$x_i = (x_{i1}, \ldots, x_{id})$ — features

$X = \big((x_1, y_1), (x_2, y_2), \ldots, (x_\ell, y_\ell)\big)$ — training set

$a(x)$ — model, hypothesis

$$x \longrightarrow a(x) \longrightarrow y^{pred}$$

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Regression and classification

$y_i \in \mathbb{R}$ — regression task

- Salary prediction
- Movie rating prediction

Regression and classification

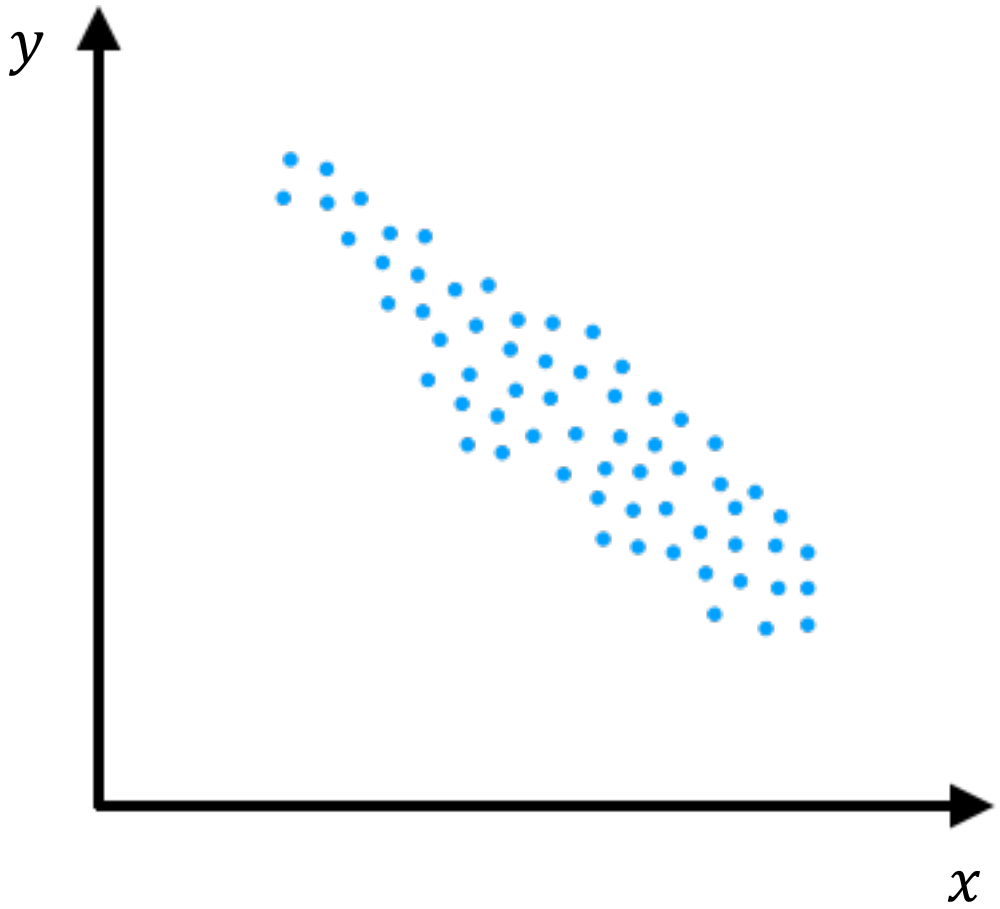
$y_i \in \mathbb{R}$ — regression task

- Salary prediction
- Movie rating prediction

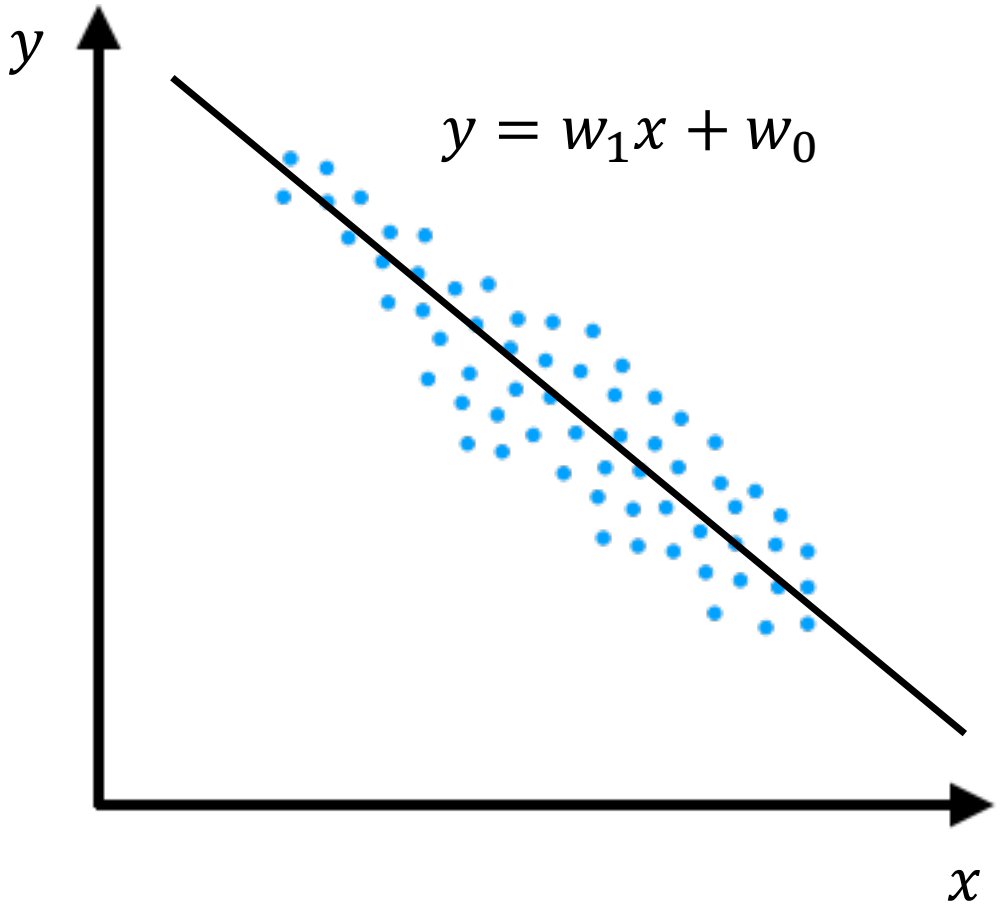
y_i belongs to a finite set — classification task

- Object recognition
- Topic classification

Linear model for regression example



Linear model for regression example



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Linear model for regression

$$a(x) = b + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$$

- $w_1, \ldots, w_d$ — coefficients (weights)
- b — bias
- $d + 1$ parameters
- To make it simple: there's always a constant feature

Linear model for regression

Vector notation:

$$a(x) = w^T x$$

For a sample X:

$$a(X) = Xw$$

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{\ell 1} & \cdots & x_{\ell d} \end{pmatrix}$$

Loss function

How to measure model quality?

Mean squared error:

$$L(w) = \frac{1}{\ell}\sum_{i=1}^{\ell}(w^T x_i - y_i)^2$$

$$= \frac{1}{\ell}\|Xw - y\|^2$$

Training a model

Fitting a model to training data:

$$L(w) = \frac{1}{\ell} \|Xw - y\|^2 \to \min_w$$

Training a model

Fitting a model to training data:

$$L(w) = \frac{1}{\ell}\|Xw - y\|^2 \to \min_{w,}$$

Exact solution:

$$w = (X^T X)^{-1} X^T y$$

But inverting a matrix is hard for high-dimensional data!

Summary

- Linear models are very simple
- MSE can be used as a loss function
- There is an analytical solution, but we need more generic and scalable learning method

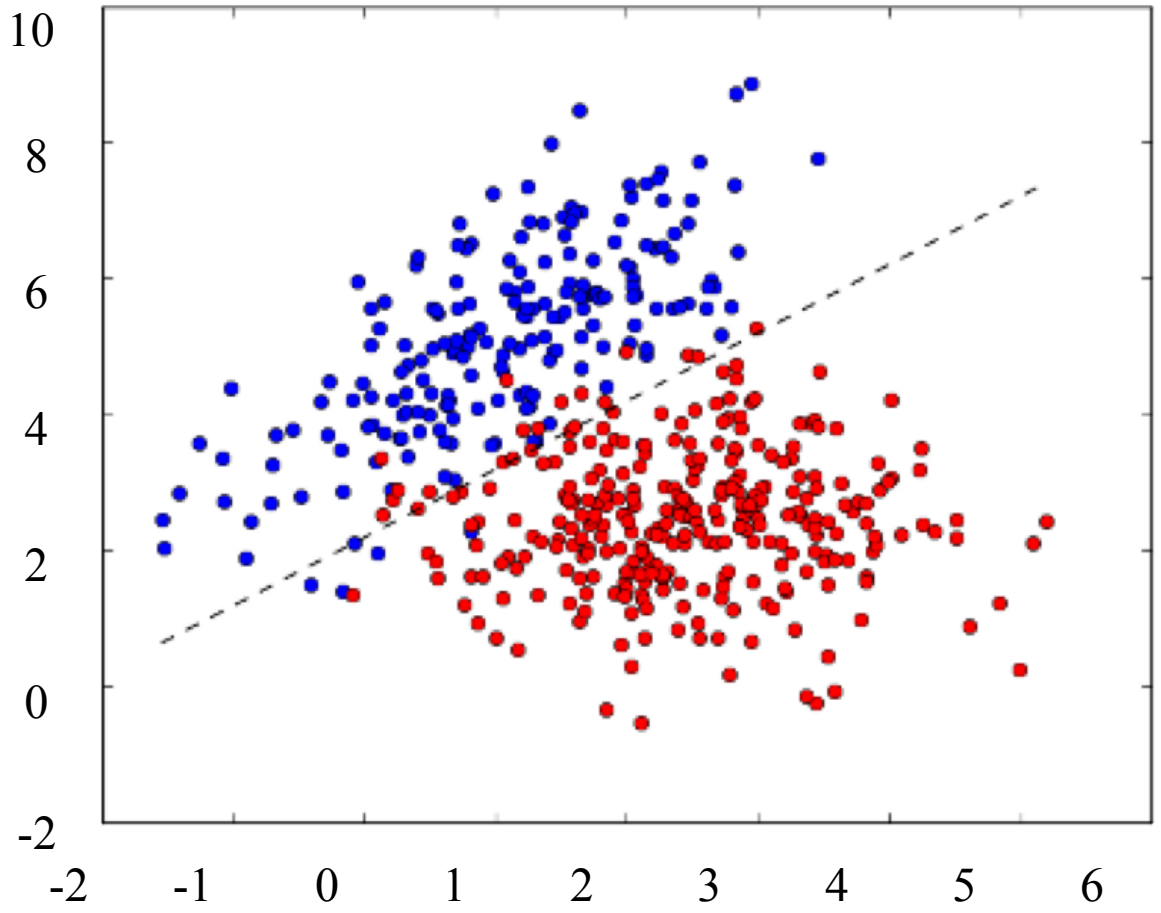
Linear model for classification

Binary classification ($y \in \{-1, 1\}$):

$$a(x) = \text{sign}(w^T x)$$

Number of parameters: d ($w \in \mathbb{R}^d$)

Linear model for classification example



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Linear model for classification

Multi-class classification ($y \in \{1, \dots, K\}$):

$$a(x) = \arg \max_{k \in \{1,\dots,K\}} \left(w_k^T x\right)$$

Number of parameters: K*d ($w_k \in \mathbb{R}^d$)

Example:

$z = (7, -7.5, 10)$ — scores

$a(x) = 3$

Classification loss

Classification accuracy:

$$\frac{1}{\ell}\sum_{i=1}^{\ell}[a(x_i) = y_i]$$

- Not differentiable
- Doesn't assess model confidence

[P] — Iverson bracket:

$$[P] = \begin{cases} 1, & P \text{ is true} \\ 0, & P \text{ is false} \end{cases}$$

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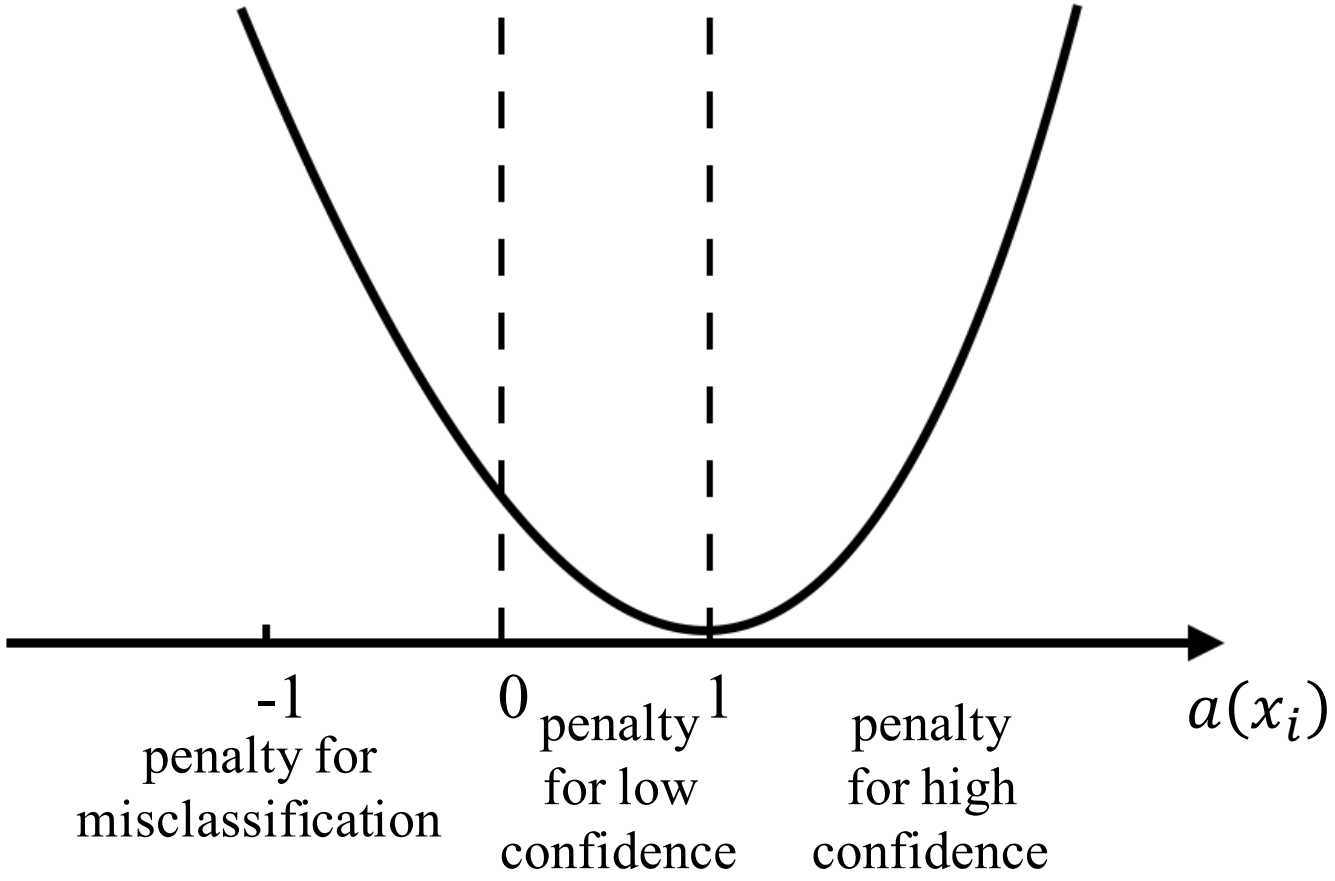
Classification loss

Consider an example x_i such that $y_i = 1$

Squared loss: $(w^T x_i - 1)^2$



Class probabilities

Class scores (**logits**) from a linear model:

$$z = (w_1^T x, \dots, w_K^T x)$$

$$(e^{z_1}, \dots, e^{z_K})$$

$$\sigma(z) = \left(\frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}}, \dots, \frac{e^{z_K}}{\sum_{k=1}^{K} e^{z_k}} \right)$$

(softmax transform)

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Softmax

$$\sigma(z) = \left(\frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}}, \cdots, \frac{e^{z_K}}{\sum_{k=1}^{K} e^{z_k}} \right)$$

Example:

$$z = (7, -7.5, 10)$$

$$\sigma(z) \approx (0.05, 0, 0.95)$$

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Loss function

Predicted class probabilities (model output):

$$\sigma(z) = \left(\frac{e^{z_1}}{\sum_{k=1}^{K} e^{z_k}}, \dots, \frac{e^{z_K}}{\sum_{k=1}^{K} e^{z_k}} \right)$$

Target values for class probabilities:

$$p = ([y = 1], \dots, [y = K])$$

Similarity between z and p can be measured by the cross-entropy:

$$-\sum_{k=1}^{K} [y = k] \log \frac{e^{z_k}}{\sum_{j=1}^{K} e^{z_j}} = -\log \frac{e^{z_y}}{\sum_{j=1}^{K} e^{z_j}}$$

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Cross-entropy examples

Suppose $K = 3$ and $y = 1$:

- $-1 * \log 1 - 0 * \log 0 - 0 * \log 0 = 0$
- $-1 * \log 0.5 - 0 * \log 0.25 - 0 * \log 0.25 \approx 0.693$
- $-1 * \log 0 - 0 * \log 1 - 0 * \log 0 = +\infty$

Cross-entropy for classification

Cross-entropy is differentiable and can be used as a loss function:

$$L(w,b) = -\sum_{i=1}^{\ell}\sum_{k=1}^{K}[y_i = k]\log\frac{e^{w_k^T x_i}}{\sum_{j=1}^{K} e^{w_j^T x_i}}$$

$$= -\sum_{i=1}^{\ell}\log\frac{e^{w_{y_i}^T x_i}}{\sum_{j=1}^{K} e^{w_j^T x_i}} \to \min_w$$

Summary

- Linear models can be easily generalized for classification tasks
- There are lots of loss functions for classification
- Cross-entropy is one of the most popular

Loss functions

Linear regression and MSE:

$$L(w) = \frac{1}{\ell} \|Xw - y\|^2$$

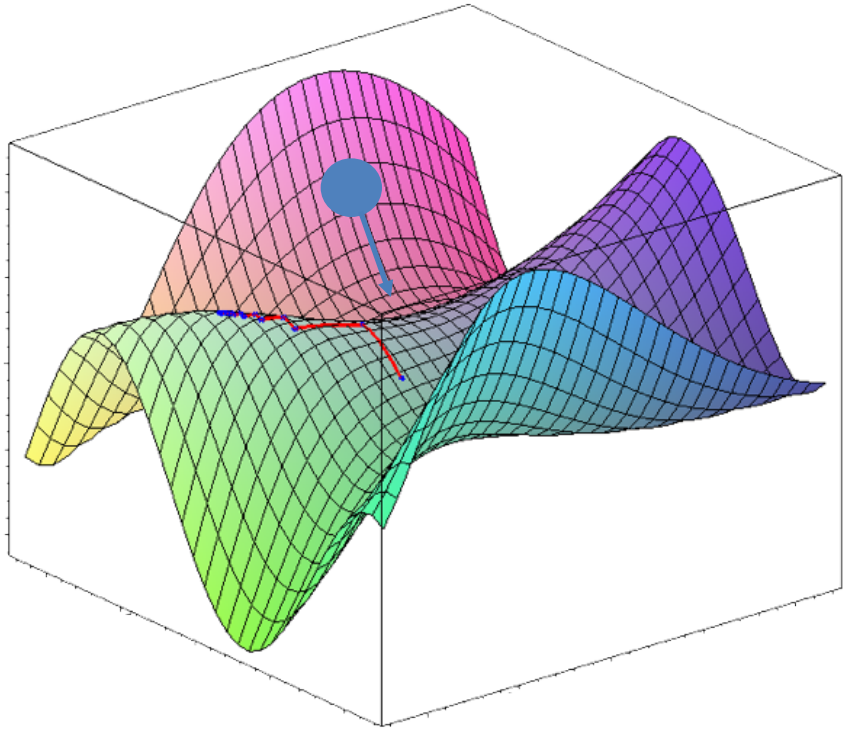
Linear classification and cross-entropy:

$$L(w) = -\sum_{i=1}^{\ell} \sum_{k=1}^{K} [y_i = k] \log \frac{e^{w_k^T x_i}}{\sum_{j=1}^{K} e^{w_j^T x_i}}$$

Gradient descent

Optimization problem: $L(w) \to \min_w$

Suppose we have some approximation w^0 — how to refine it?



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Gradient descent

Optimization problem: $L(w) \to \min_w$

w^0 — initialization

$\nabla L(w^0) = \left(\frac{\partial L(w^0)}{\partial w_1}, \dots, \frac{\partial L(w^0)}{\partial w_n}\right)$ — gradient vector

- Points in the direction of the steepest slope at w^0
- The function has fastest decrease rate in the direction of negative gradient

Gradient descent

Optimization problem: $L(w) \to \min_w$

w^0 — initialization

$\nabla L(w^0) = \left(\frac{\partial L(w^0)}{\partial w_1}, \ldots, \frac{\partial L(w^0)}{\partial w_n}\right)$ — gradient vector

$w^1 = w^0 - \eta_1 \nabla L(w^0)$ — gradient step

Gradient descent

Optimization problem: $L(w) \to \min_w$

w^0 — initialization

while True:

$$w^t = w^{t-1} - \eta_t \nabla L(w^{t-1})$$

if $\|w^t - w^{t-1}\| < \epsilon$ then break

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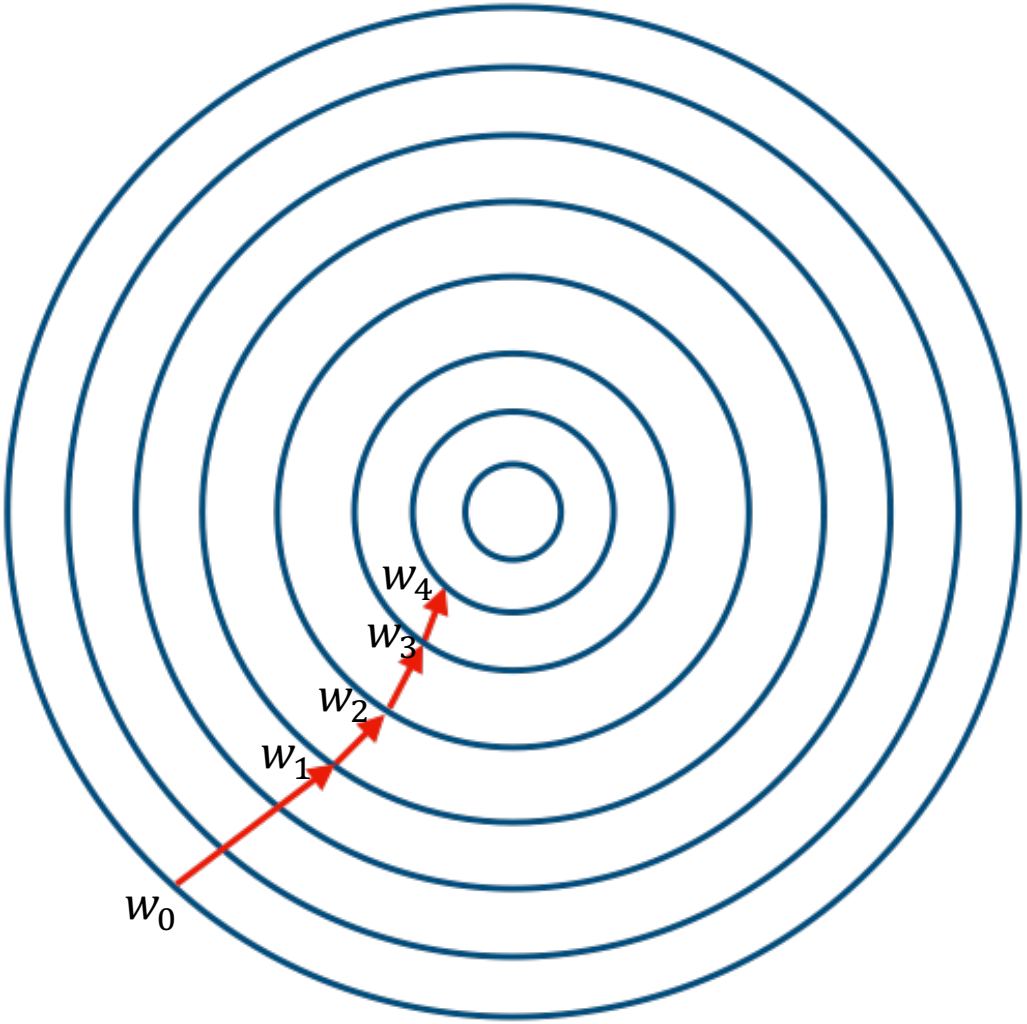
Gradient descent



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Gradient descent

Lots of heuristics:

- How to initialize w^0
- How to select step size η_t
- When to stop
- How to approximate gradient $\nabla L(w^{t-1})$

Gradient descent for MSE

Linear regression and MSE:

$$L(w) = \frac{1}{\ell} \|Xw - y\|^2$$

Derivatives:

$$\nabla L_w(w) = \frac{2}{\ell} X^T (Xw - y)$$

Gradient descent vs analytical solution

Analytical solution for MSE: $w = (X^T X)^{-1} X^T y$

Gradient descent:

- Easy to implement
- Very general, can be applied to any differentiable loss function
- Requires less memory and computations (for stochastic methods)

Summary

- Gradient descent provides a general learningframework
- Can be used both for classificationand regression tasks
- Advanced methods — in the next lectures

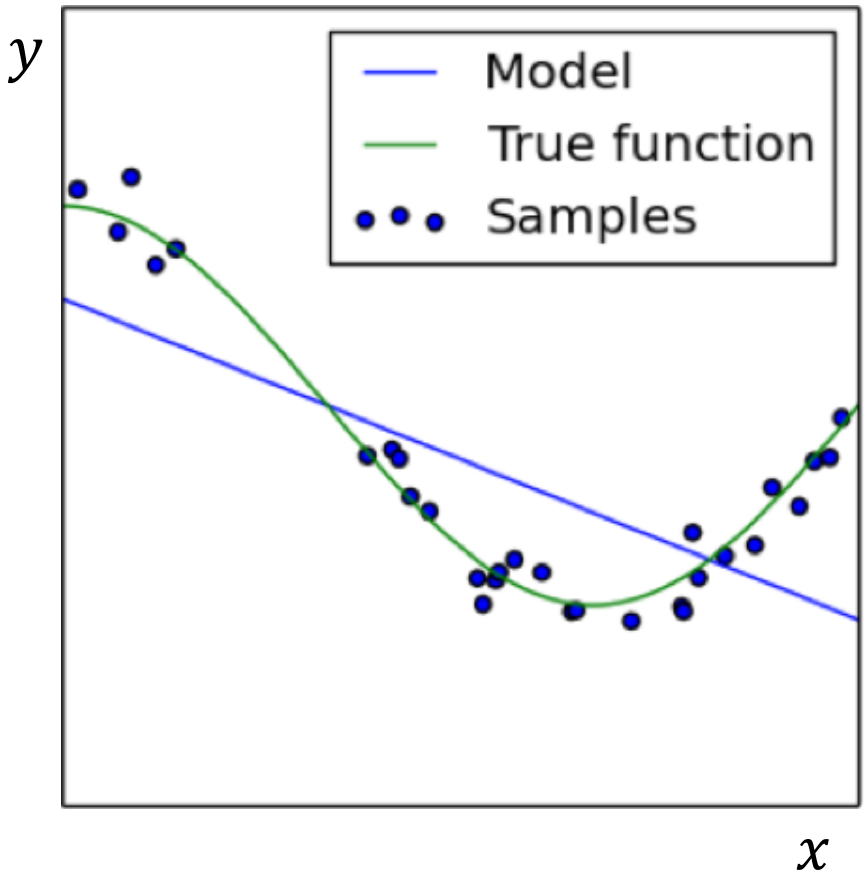
Generalization

- Consider a model with accuracy 80% on training set
- How will it perform on the new data?
- Does the model generalize well?

Underfitting and overfitting example

Training set: $X \subset \mathbb{R}$

Model: $a(x) = b + w_1 x$



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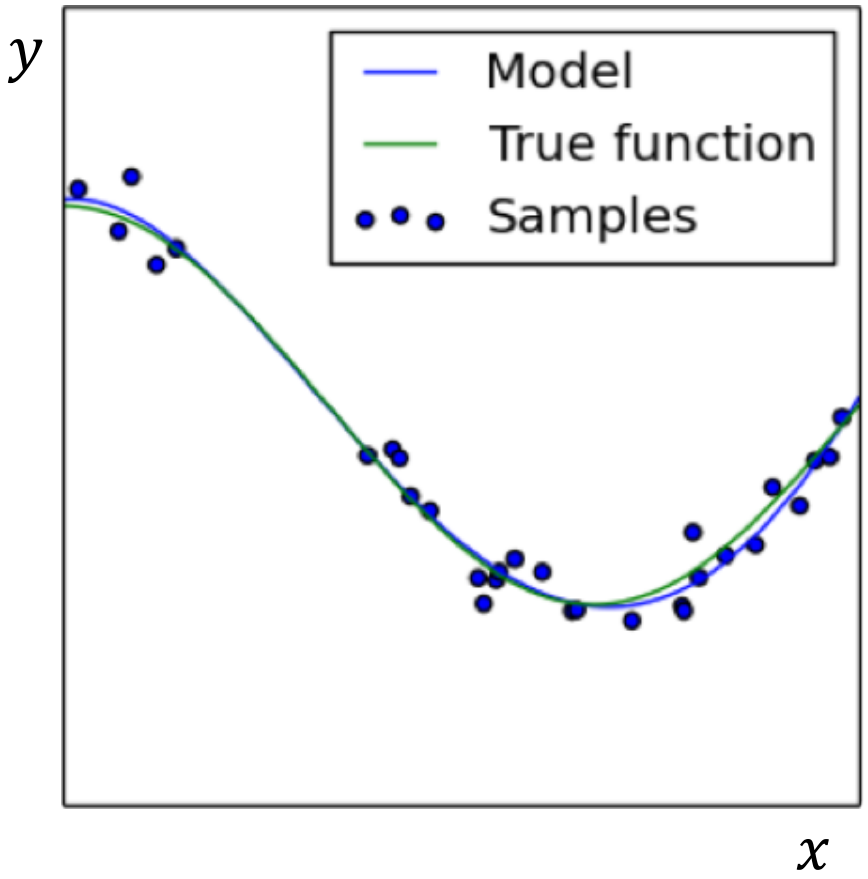
Underfitting and overfitting example

Training set: $X \subset \mathbb{R}$

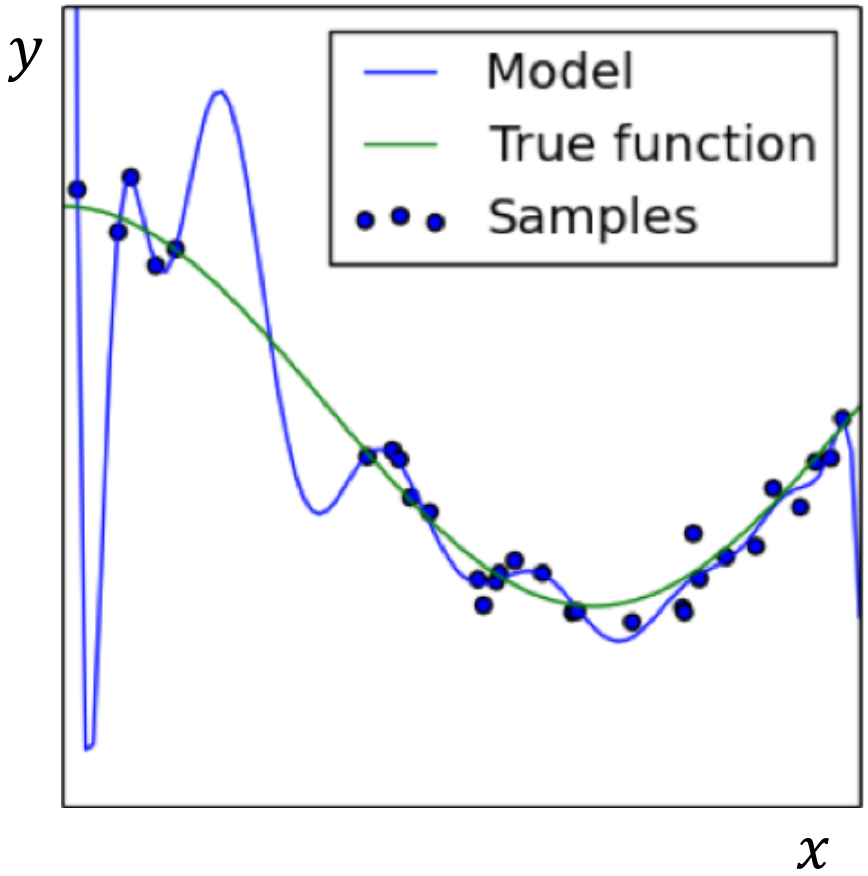
Model: $a(x) = b + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4$



Underfitting and overfitting example

Training set: $X \subset \mathbb{R}$

Model: $a(x) = b + w_1 x + w_2 x^2 + \cdots + w_{15} x^{15}$



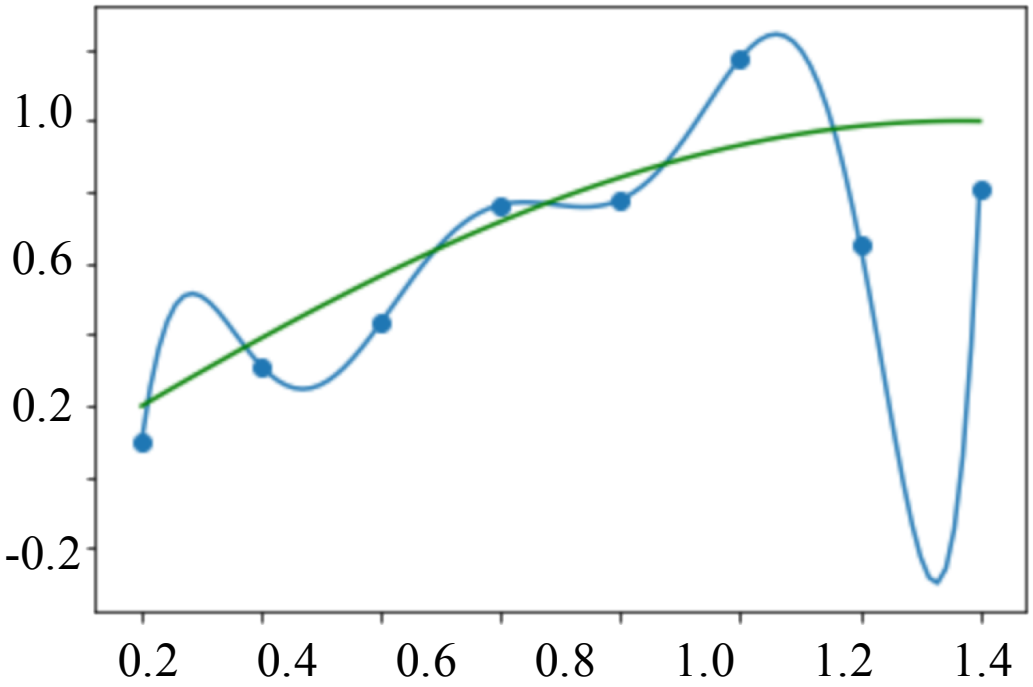
Overfitting example 2

Training set: $\{0.2, 0.4, \ldots, 1.6\}$, $y = \sin(x) + \epsilon$

Model: $a(x) = b + w_1 x + w_2 x^2 + \cdots + w_8 x^8$

Parameters: $(130.0, -525.8, \ldots, 102.6)$

Model just incorporates target into parameters!



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Holdout set

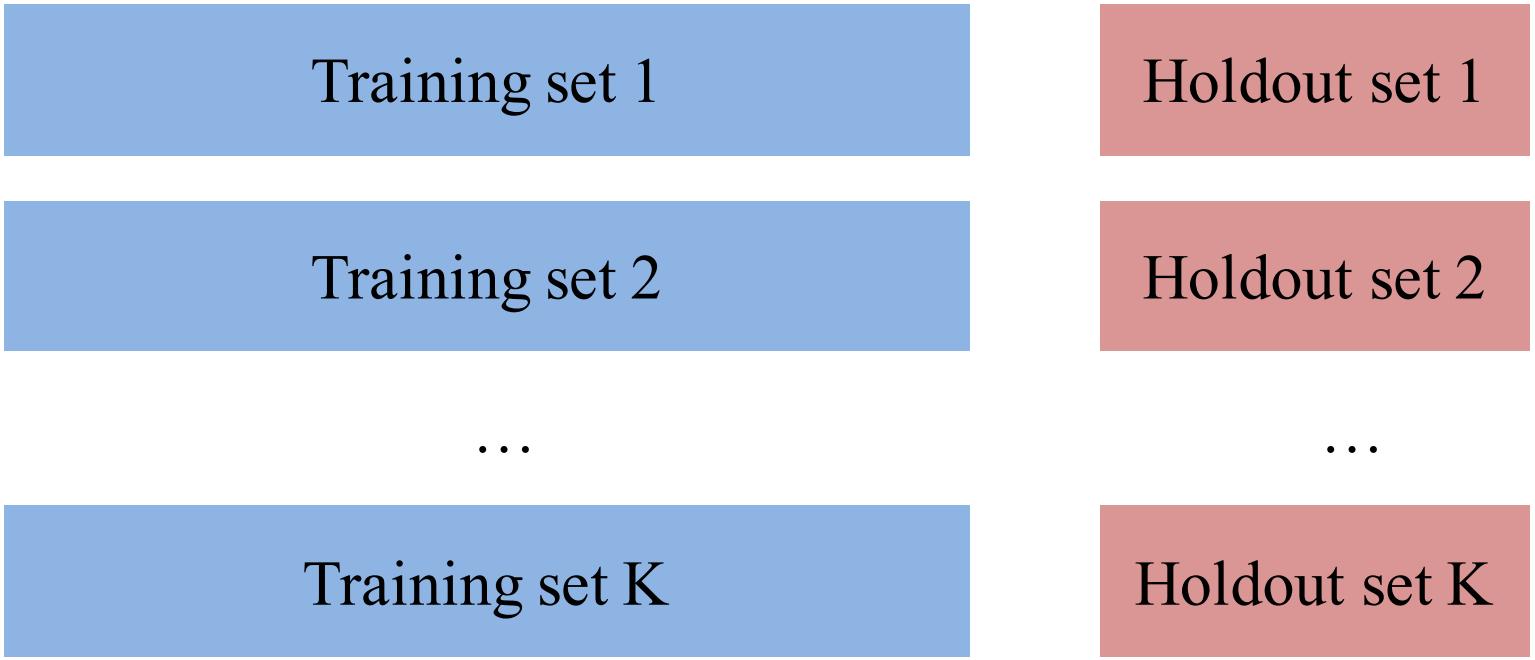
Small holdout set:

- Training set is representative
- Holdout quality has high variance

Large holdout set:

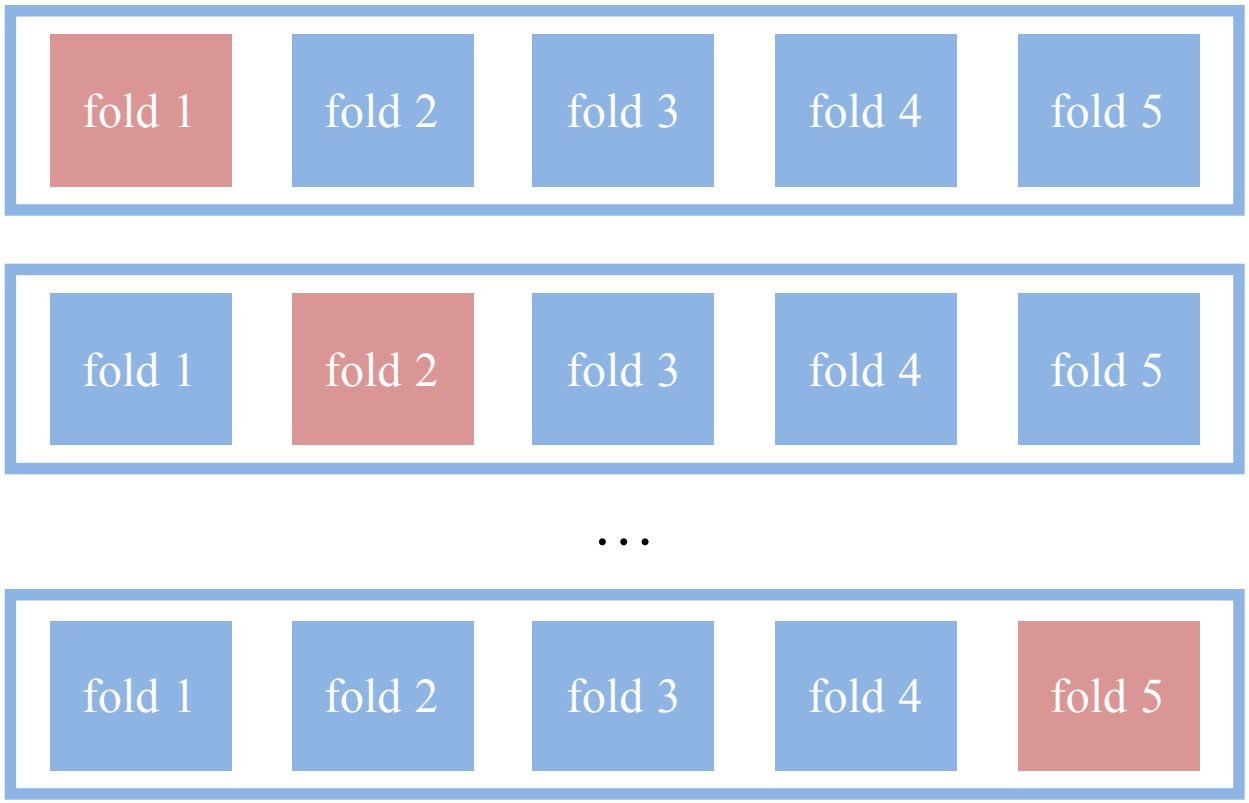
- Holdout quality has low variance
- Holdout quality has high bias

Holdout set



No guarantees that each object will be in holdout part at least once

Cross-validation



Cross-validation

- Requires to train models K times for K-fold CV
- Useful for small samples
- In deep learning holdout samples are usually preferred

Summary

- Models can easily overfit with high number of parameters
- Overfitted model just remembers target values for training set and doesn't generalize
- Holdout set or cross-validation can be used to estimate model performance on new data

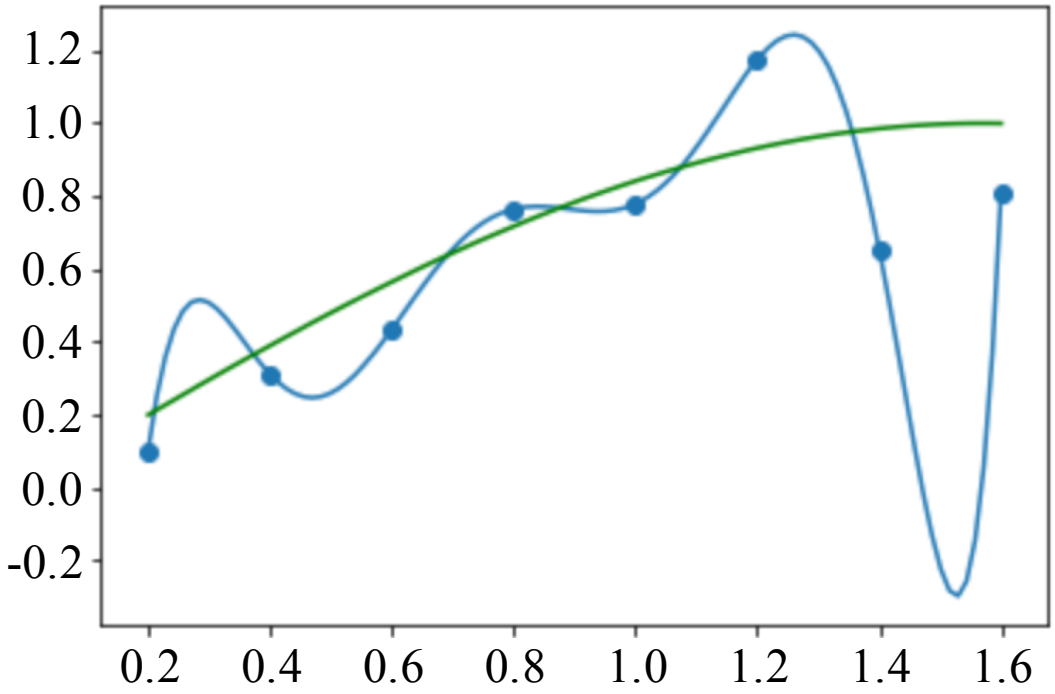
Overfitting example

Training set: $\{0.2, 0.4, \ldots, 1.6\}$, $y = \sin(x) + \epsilon$

Model: $a(x) = b + w_1 x + w_2 x^2 + \cdots + w_8 x^8$

Parameters: $(130.0, -525.8, \ldots, 102.6)$

Model just incorporates target into parameters!



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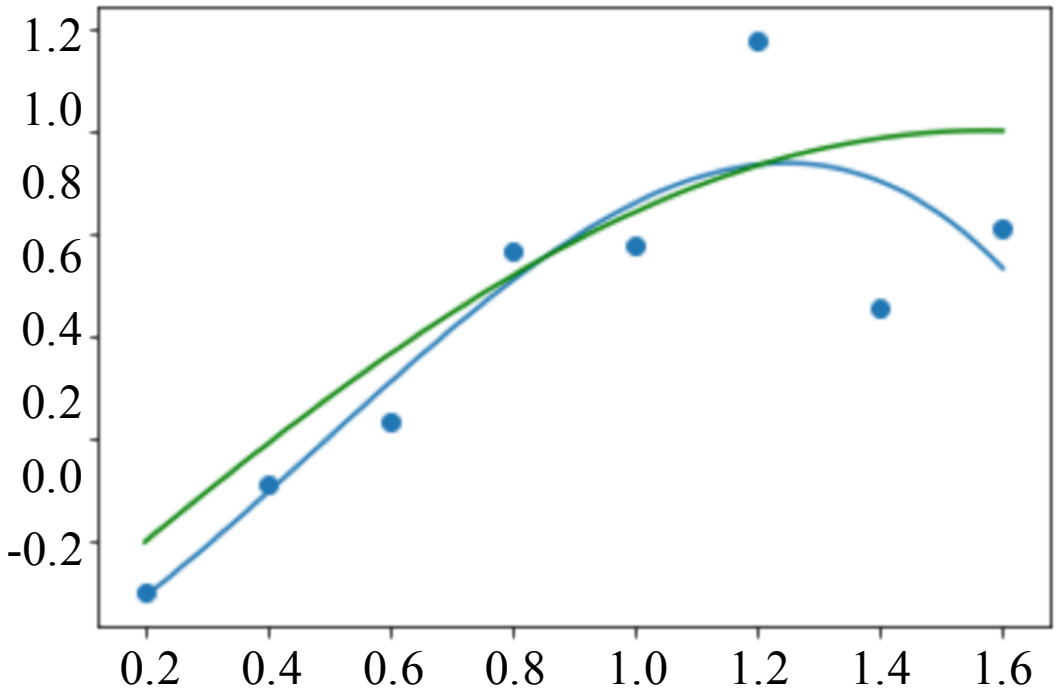
Overfitting example

Training set: $\{0.2, 0.4, \ldots, 1.6\}$, $y = \sin(x) + \epsilon$

Model: $a(x) = b + w_1 x + w_2 x^2 + w_3 x^3$

Parameters: $(0.634, 0.918, -0.626)$



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Regularization

Good model weights: $(0.634, 0.918, -0.626)$

Overfitted model weights: $(130.0, -525.8, \ldots, 102.6)$

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Weight penalty

$$L_{reg}(w) = L(w) + \lambda R(w) \to \min_{w}$$

- $L(w)$ — loss function (MSE, log-loss, etc.)
- $R(w)$ — regularizer (e.g. penalizes large weights)
- λ — regularization strength

L2 penalty

$$L_{reg}(w) = L(w) + \lambda \|w\|^2 \to \min_w$$

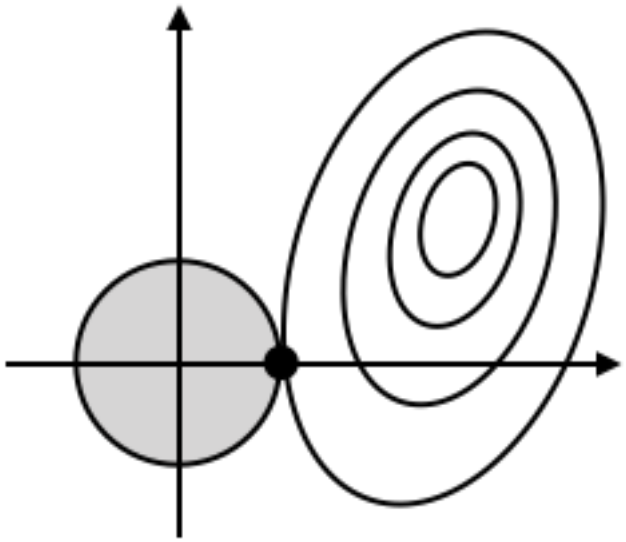
- $\|w\|^2 = \sum_{j=1}^{d} w_j^2$
- Drives all weights **closer** to zero
- Can be optimized with gradient methods

L2 penalty

$$L_{reg}(w) = L(w) + \lambda \|w\|^2 \to \min_w$$

The optimization problem is equivalent to

$$\begin{cases} L(w) \to \min\limits_w \\ \text{s.t. } \|w\|^2 \le C \end{cases}$$



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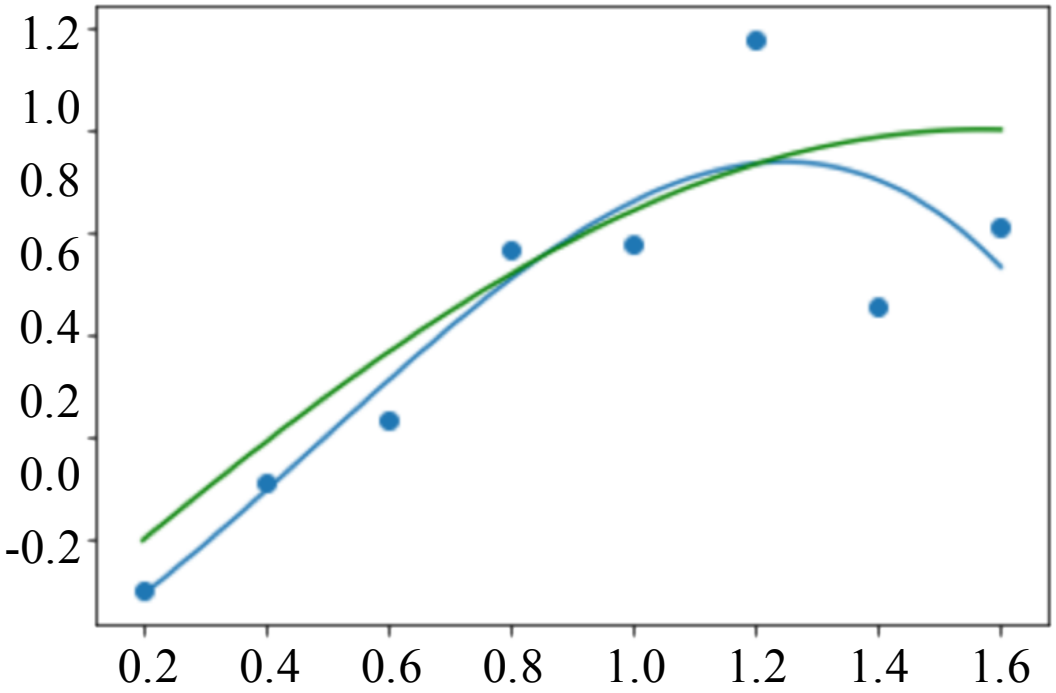
L2 penalty

$$L_{reg}(w) = L(w) + \lambda\|w\|^2 \to \min_w$$

Training set: $\{0.2, 0.4, \ldots, 1.6\}$, $y = \sin(x) + \epsilon$

Model: $a(x) = b + w_1 x + w_2 x^2 + \cdots + w_8 x^8$

Parameters: $(0.166, 0.168, 0.13, 0.075, 0.014, -0.04, -0.05, 0.018)$



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L1 penalty

$$L_{reg}(w) = L(w) + \lambda \|w\|_1 \to \min_w$$

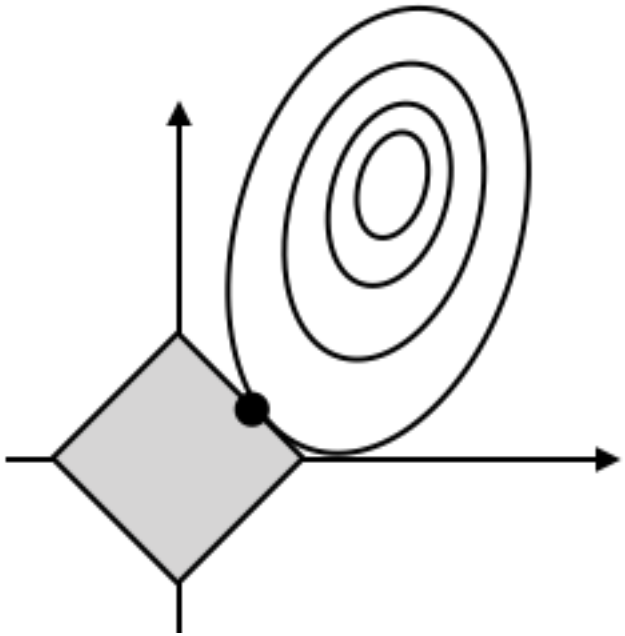
- $\|w\|_1 = \sum_{j=1}^{d} |w_j|$
- Drives some weights **exactly** to zero
- Learns sparse models
- Cannot be optimized with simple gradient methods

L1 penalty

$$L_{reg}(w) = L(w) + \lambda\|w\|_1 \to \min_w$$

The optimization problem is equivalent to

$$\begin{cases} L(w) \to \min\limits_w \\ \text{s.t. } \|w\|_1 \le C \end{cases}$$



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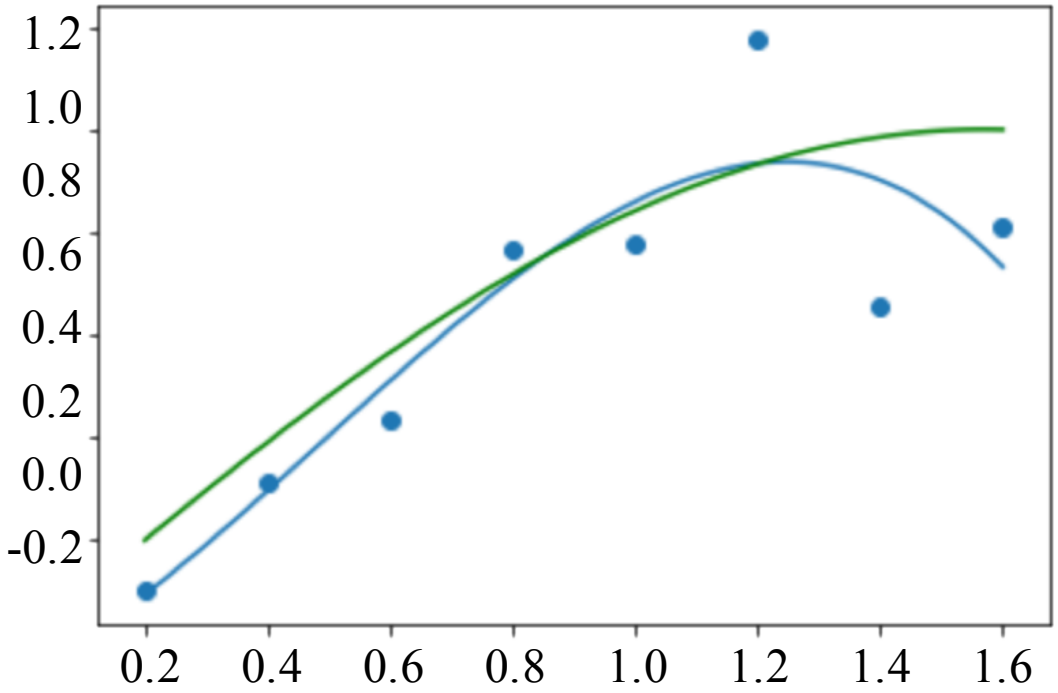
L1 penalty

$$L_{reg}(w) = L(w) + \lambda\|w\|_1 \to \min_w$$

Training set: $\{0.2, 0.4, \ldots, 1.6\}$, $y = \sin(x) + \epsilon$

Model: $a(x) = b + w_1 x + w_2 x^2 + \cdots + w_8 x^8$

Parameters: (for $\lambda = 0.01$): (0.78, 0.03, **0**, **0**, **0**, −0.016, −0.01, **0**)



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Weight Decay

L2-regularization:

$$L2_{reg}(w) = L(w) + \lambda\left|\left|w\right|\right|^2 \rightarrow \min_w$$

$$w_t = w_{t-1} - \eta\frac{\delta L}{\delta w_{t-1}}$$

Weight Decay:

$$w_t = (1 - \lambda) \cdot w_{t-1} - \eta\frac{\delta L}{\delta w_{t-1}}$$

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Other regularization techniques

- Dimensionality reduction
- Data augmentation
- Dropout
- Early stopping
- Collect more data

Summary

- One should restrict model complexity to prevent overfitting
- Common approach: penalize large weights
- Other approaches: next modules

Stochastic gradient descent

Gradient descent

Optimization problem:

$$L(w) = \sum_{i=1}^{\ell} L(w; x_i, y_i) \to \min_w$$

w^0 — initialization

while True:

$$w^t = w^{t-1} - \eta_t \nabla L(w^{t-1})$$

if $\|w^t - w^{t-1}\| < \epsilon$ then break

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Gradient descent

Mean squared error:

$$\nabla L(w) = \frac{1}{\ell}\sum_{i=1}^{\ell} \nabla(w^T x_i - y_i)^2$$

- ℓ gradients should be computed on each step
- If the dataset doesn't fit into the memory, it should be read from the disk on every GD step

Stochastic gradient descent

Optimization problem:

$$L(w) = \sum_{i=1}^{\ell} L(w; x_i, y_i) \to \min_w$$

w^0 — initialization

while True:

i = random index between 1 and ℓ

$$w^t = w^{t-1} - \eta_t \nabla L(w^{t-1}; x_i; y_i)$$

if $\|w^t - w^{t-1}\| < \epsilon$ then break

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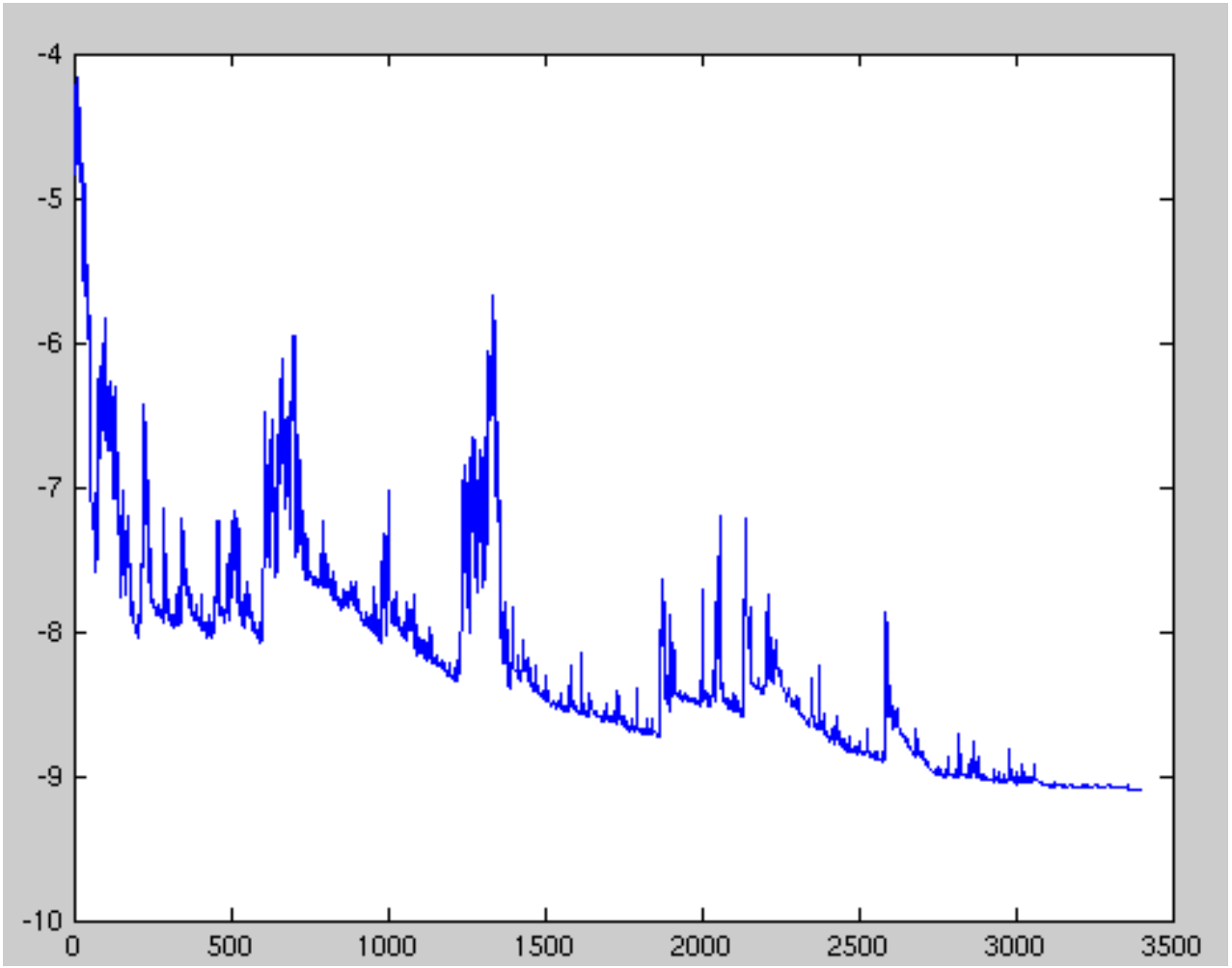
Stochastic gradient descent



Joe pharos, https://en.wikipedia.org/wiki/Stochastic_gradient_descent

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Stochastic gradient descent

- Noisy updates lead to fluctuations
- Needs only one example on each step
- Can be used in online setting
- Learning rate η_t should be chosen very carefully

Mini-batch gradient descent

Optimization problem:

$$L(w) = \sum_{i=1}^{\ell} L(w; x_i, y_i) \to \min_w$$

w^0 — initialization

while True:

$i_1, \dots, i_m$ = random indices between 1 and ℓ

$w^t = w^{t-1} - \eta_t \frac{1}{m} \sum_{j=1}^{m} \nabla L\left(w^{t-1}; x_{i_j}; y_{i_j}\right)$

if $\|w^t - w^{t-1}\| < \epsilon$ then break

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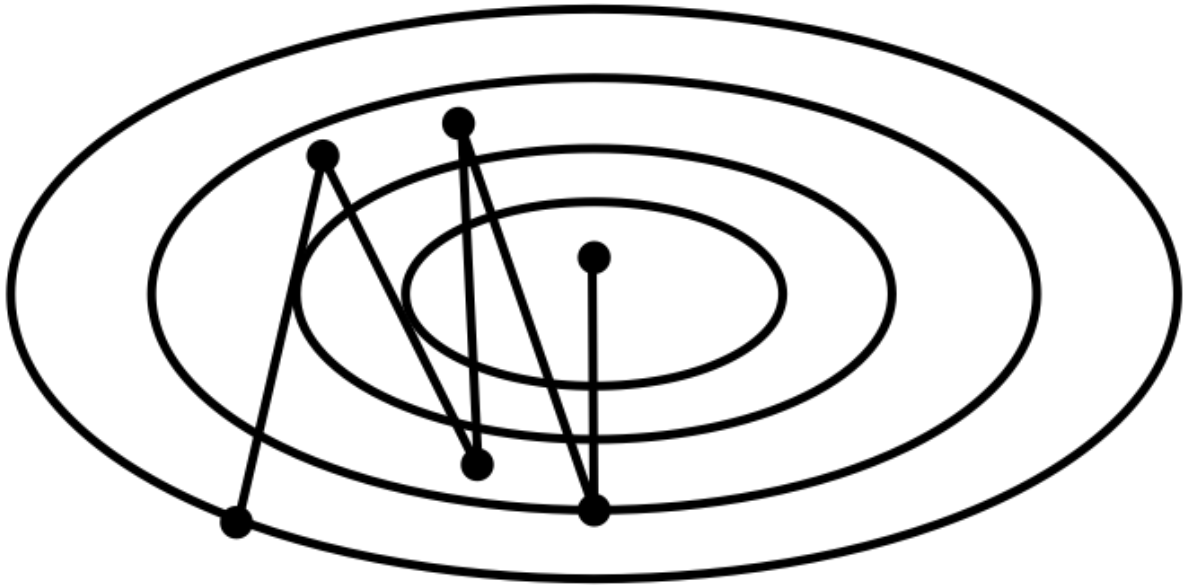
Mini-batch gradient descent

- Still can be used in online setting
- Reduces the variance of gradient approximations
- Learning rate η_t should be chosen carefully

Difficult function



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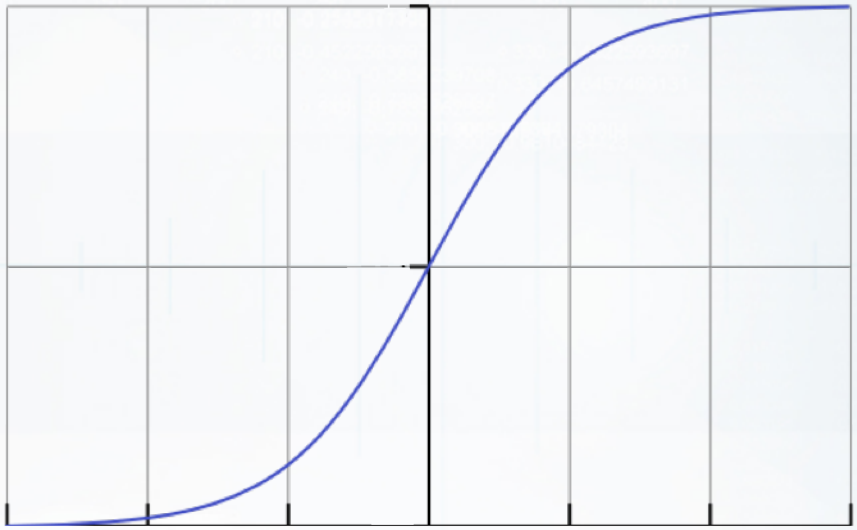
Summary

- Gradient descent is infeasible for large training sets
- Stochastic and mini-batch descents use gradient approximations to speed up computations
- Learning rate is quite hard to select
- Methods can be optimized for difficult functions

Multilayer perceptron

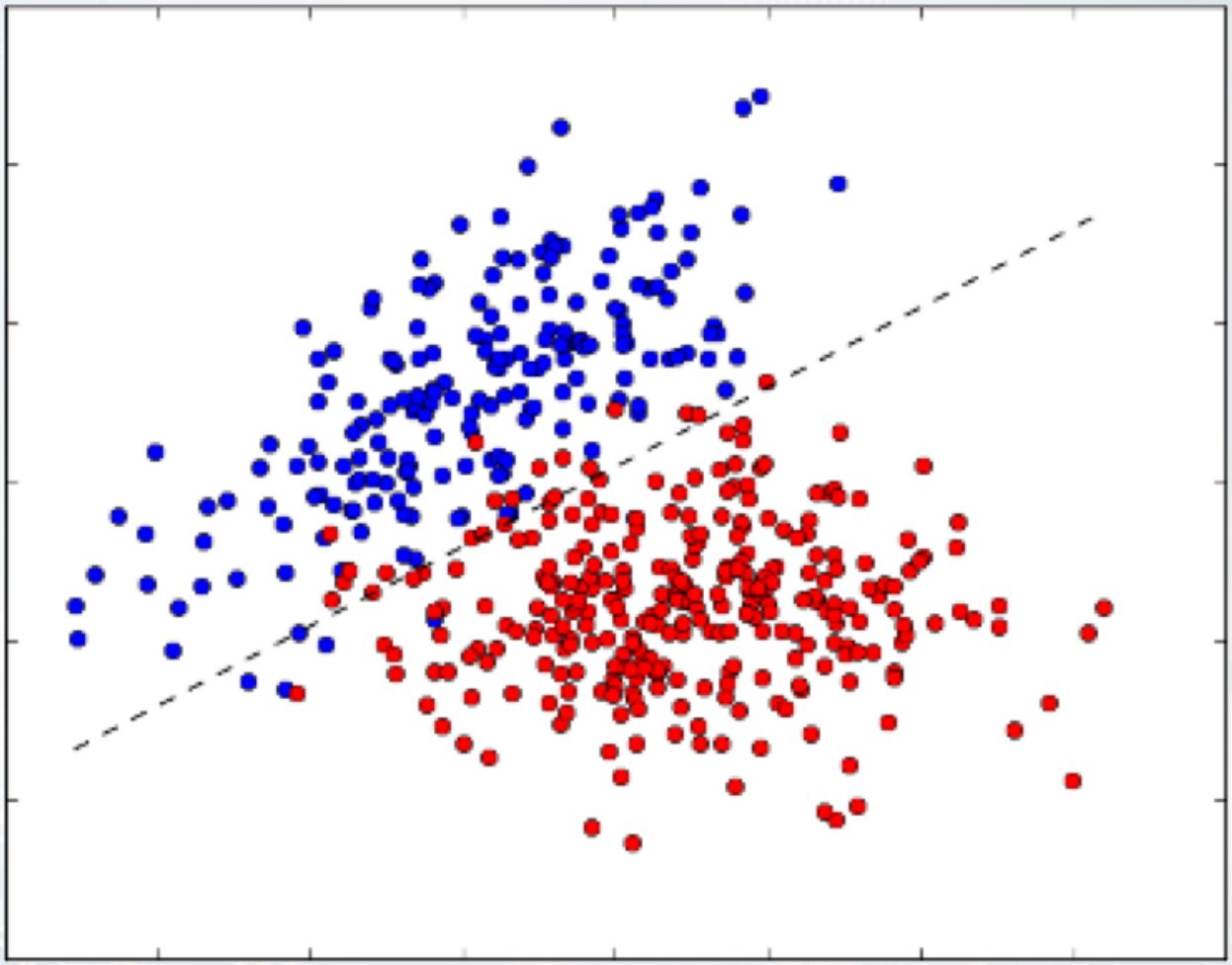
Recap: linear model

$W \cdot x + b \rightarrow$  $\rightarrow P(y = +1|x)$

x - features vector

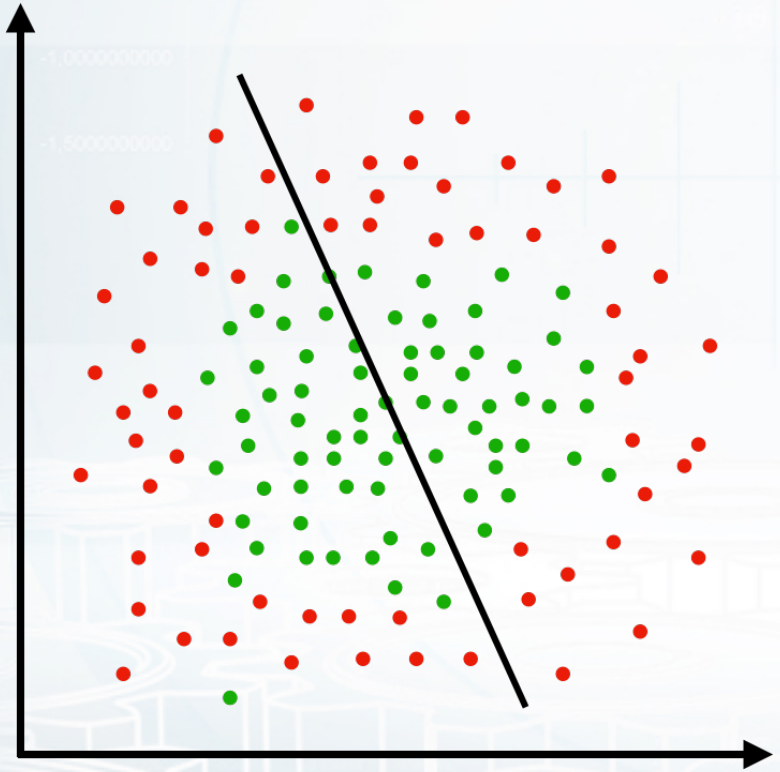
W, b - model slope and intercept

Linear dependency

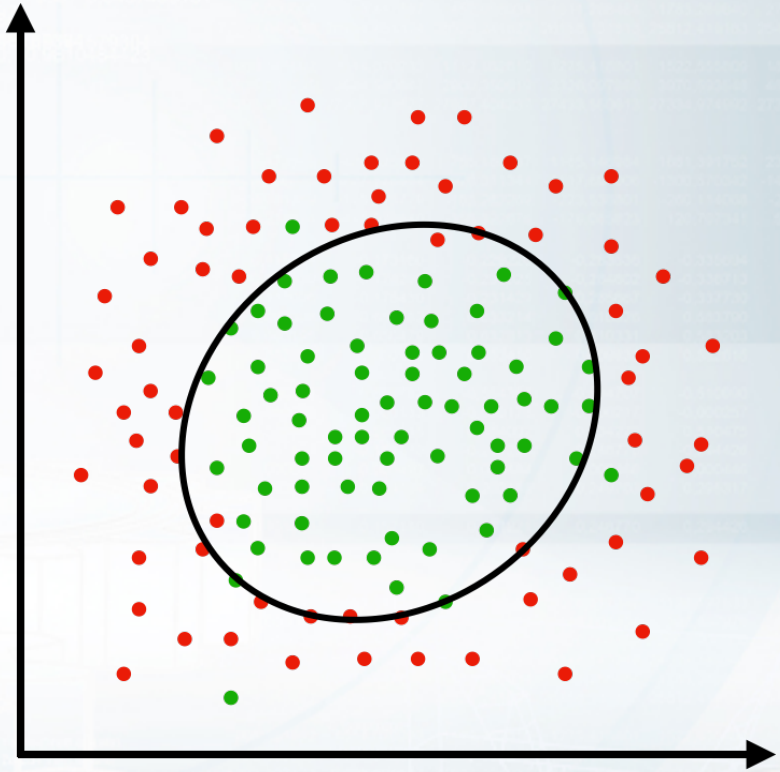


Nonlinear dependencies

What we have



What we want



Somewhat nonlinear dependencies

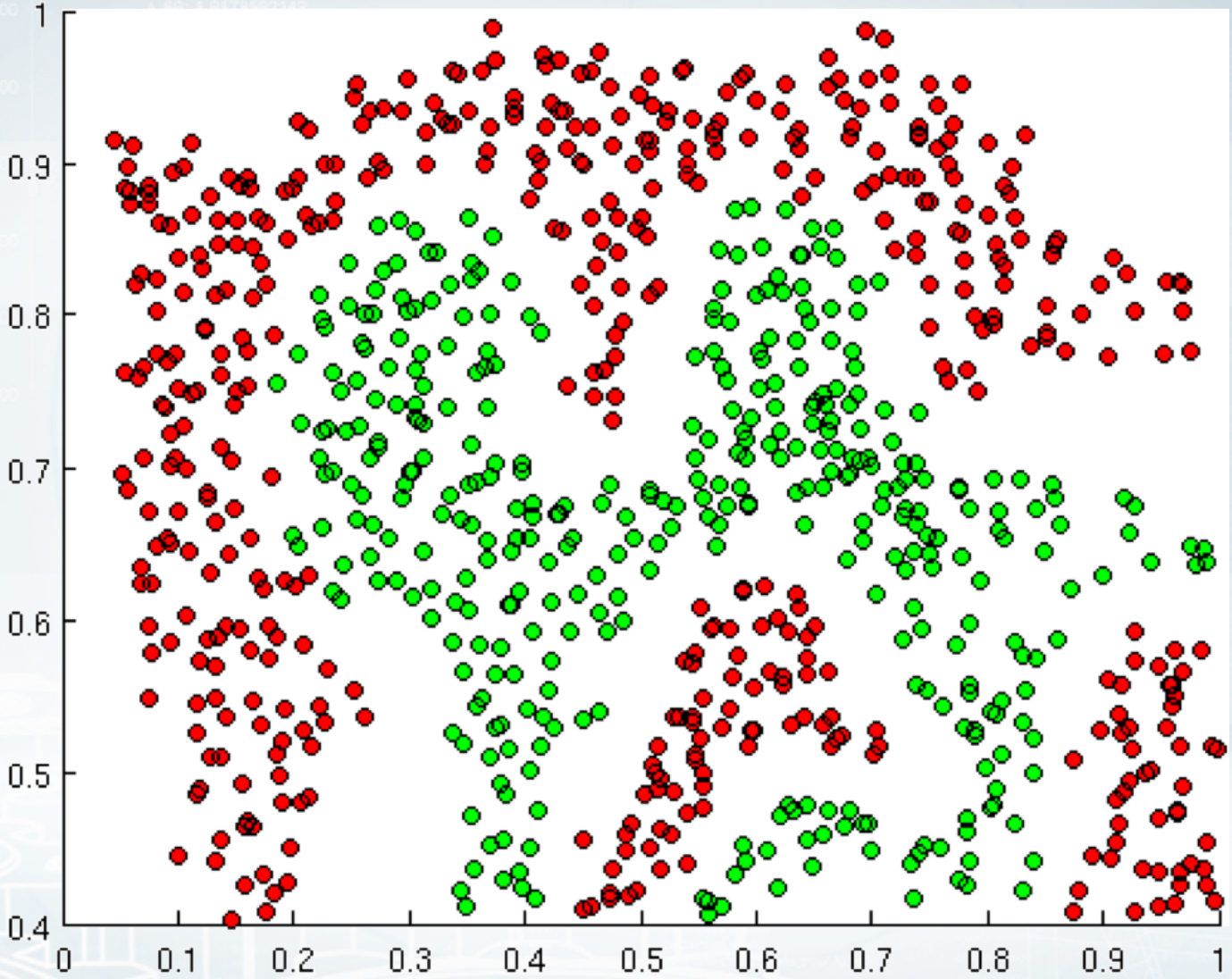
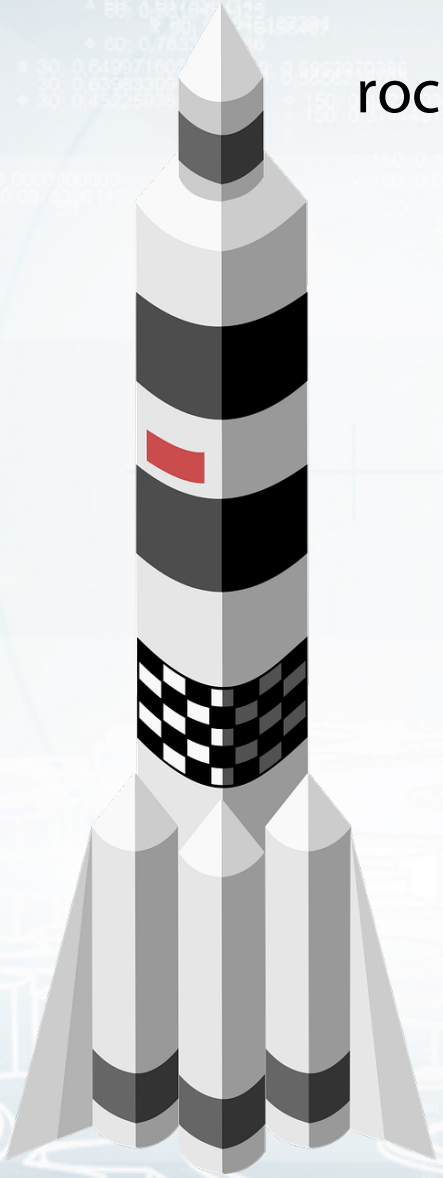


Image: Andrew Ng

Extremely nonlinear dependencies

rocket



cat

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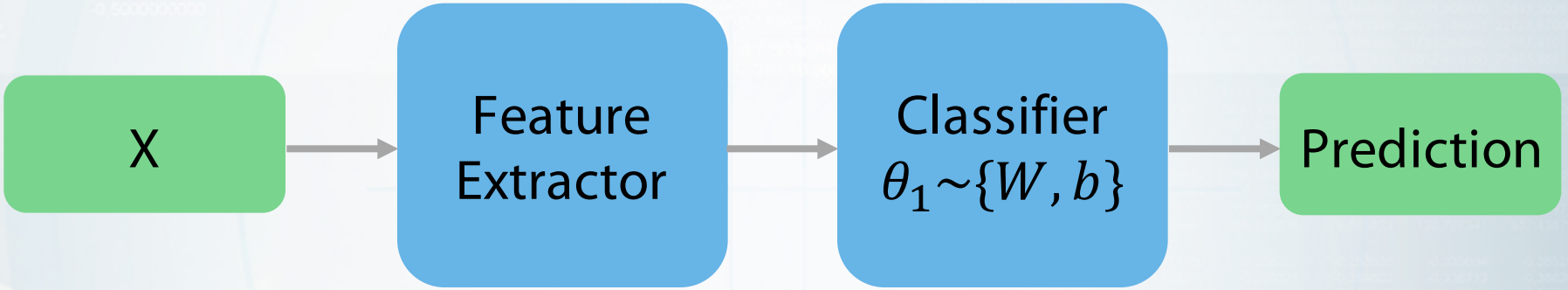
Extremely nonlinear dependencies



Feature extraction

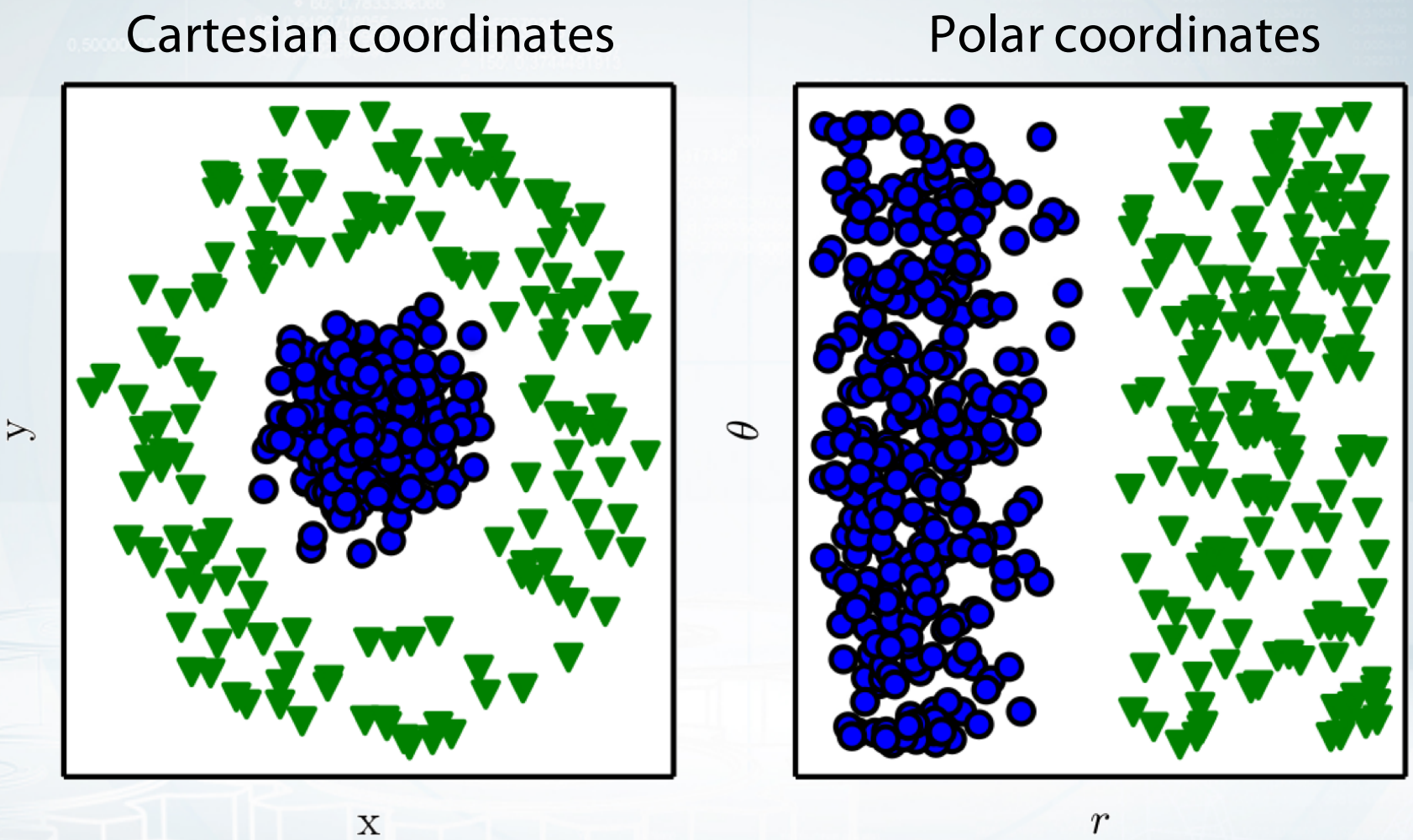
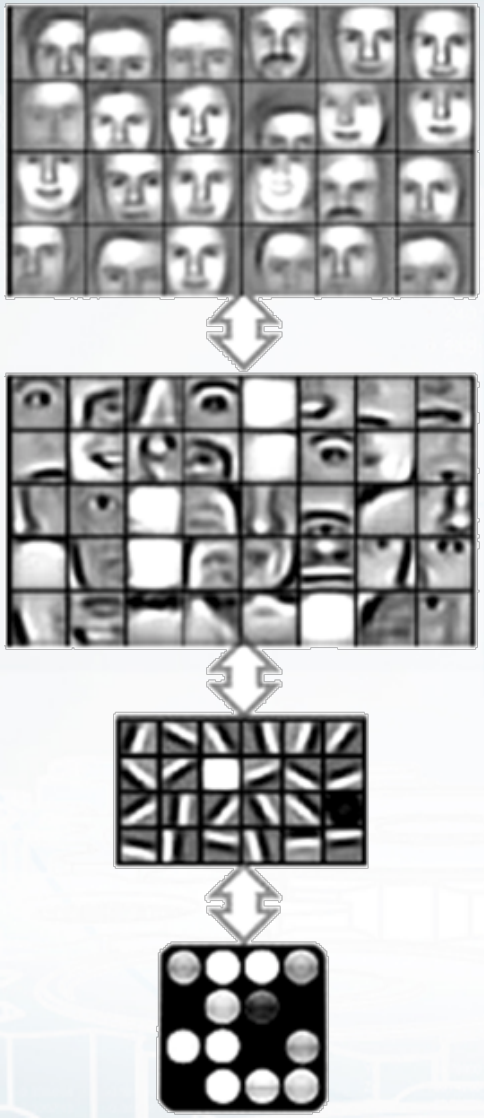


Image: Ian Goodfellow et al.



Discrete Choices

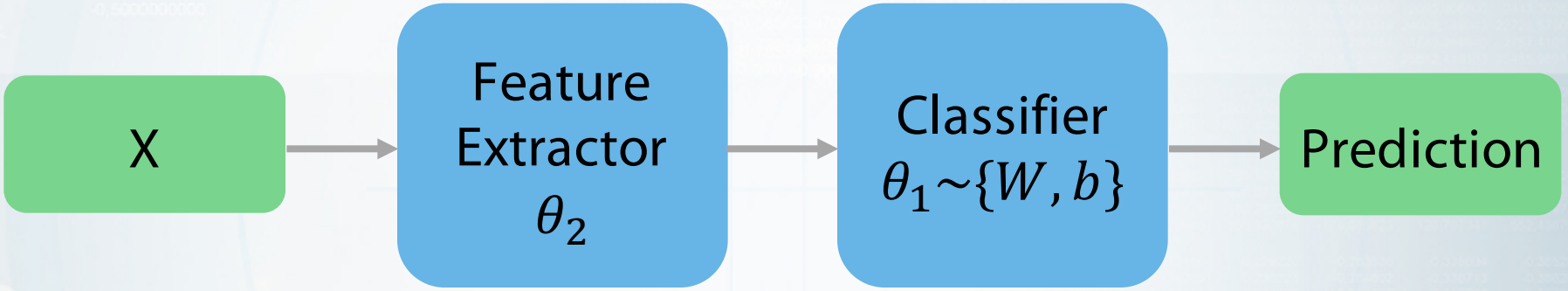
Layer 2 Features

Layer 1 Features

Original Data

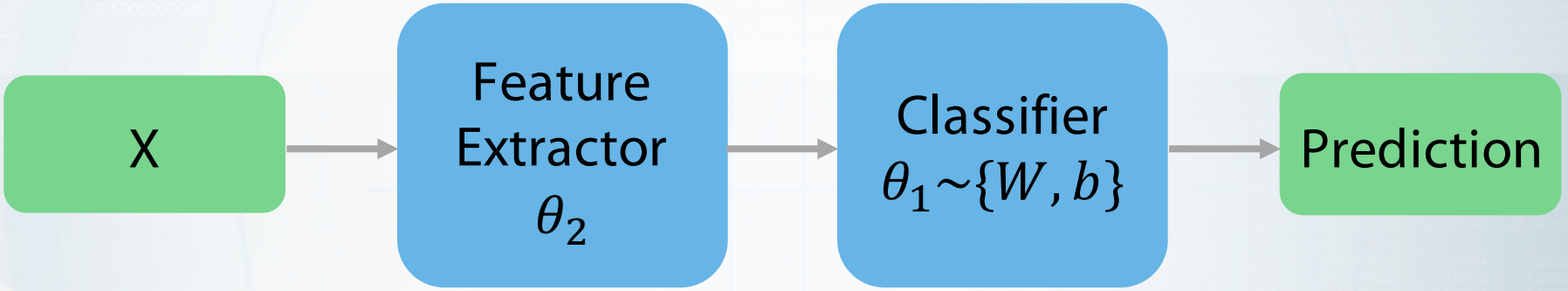
Image: Alex Burnap et al.

Feature extraction



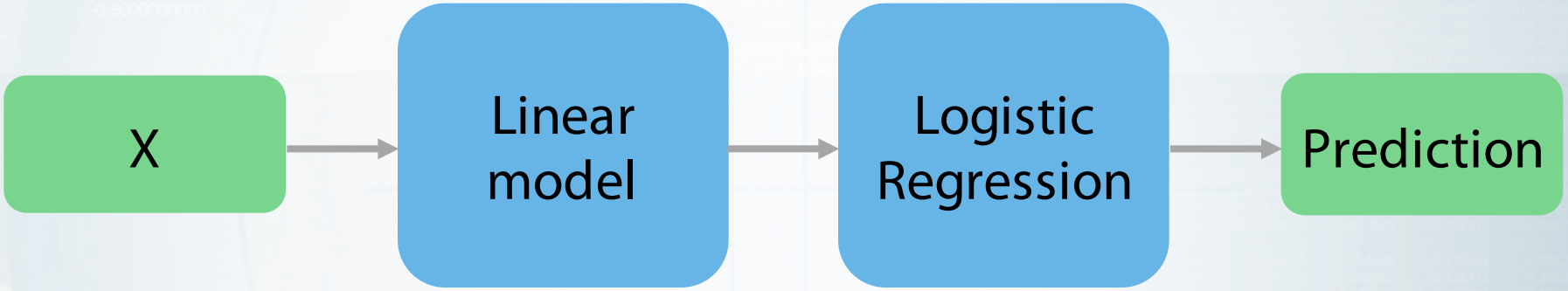
Training: manual $\underset{\theta_1}{\operatorname{argmin}} L\big(y, P(y \mid x)\big)$

Can it be done automatically?



Training: ? $\underset{\theta_1}{\operatorname{argmin}} L\big(y, P(y \mid x)\big)$

Try linear



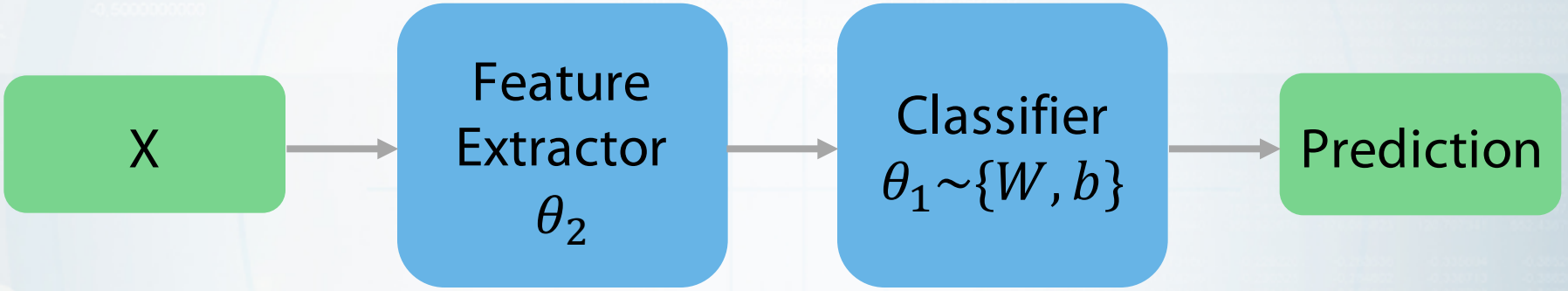
$$h_j = \sum_i w_{ij}^h x_i + b_j^h \qquad y_{\text{pred}} = \sigma\left(\sum_j w_j^o h_j + b^o\right)$$

$$j \in \{1,2,\ldots,n\}$$

Training:

$$\underset{w^h, w^0, b^h, b^0}{\text{argmin}} \; L\big(y, P(y \mid x)\big)$$

Can it be done automatically?



Training: ? $\underset{\theta_1}{\operatorname{argmin}} L\big(y, P(y \mid x)\big)$

Answer: No

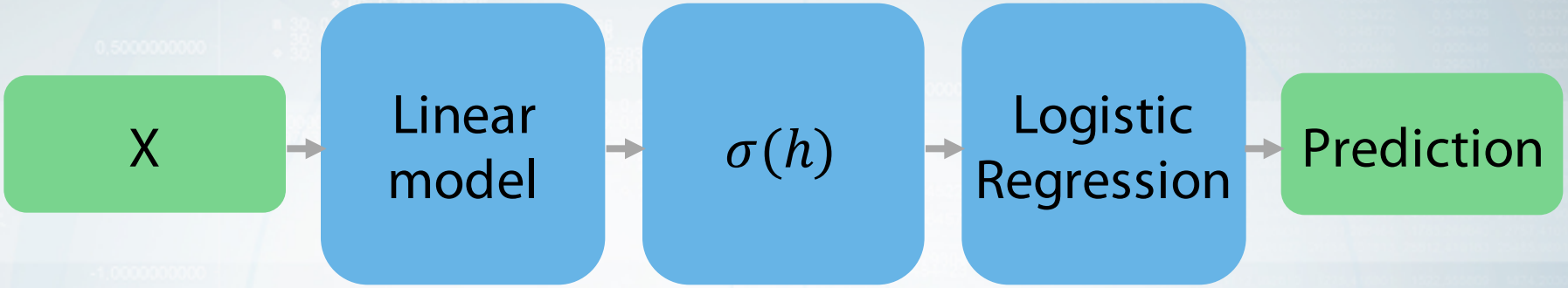
A combination of linear models is a linear model

$$P(y \mid x) = \sigma\left(\sum_j w_j^o \left(\sum_i w_{ij}^h x_i + b_j^h\right) + b^o\right)$$

$$w'_i = \sum_j w_j^o w_{ij}^h \qquad b' = \sum_j w_j^o b_j^h + b^o$$

$$P(y \mid x) = \sigma\left(\sum_i w'_i x_i + b'\right)$$

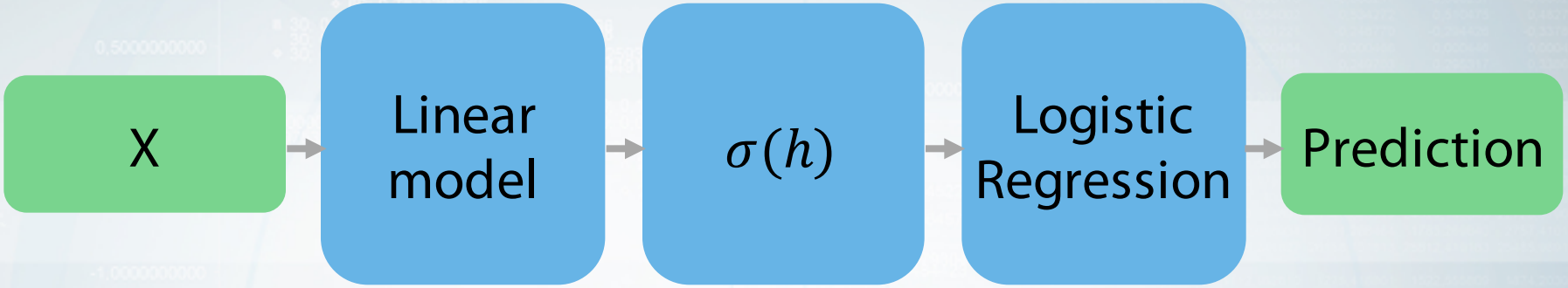
Nonlinearity



$$h_j = \sigma\left(\sum_i w_{ij}^h x_i + b_j^h\right) \qquad y_{\text{pred}} = \sigma\left(\sum_j w_j^o h_j + b^o\right)$$

$$j \in \{1,2,\ldots,n\}$$

Nonlinearity

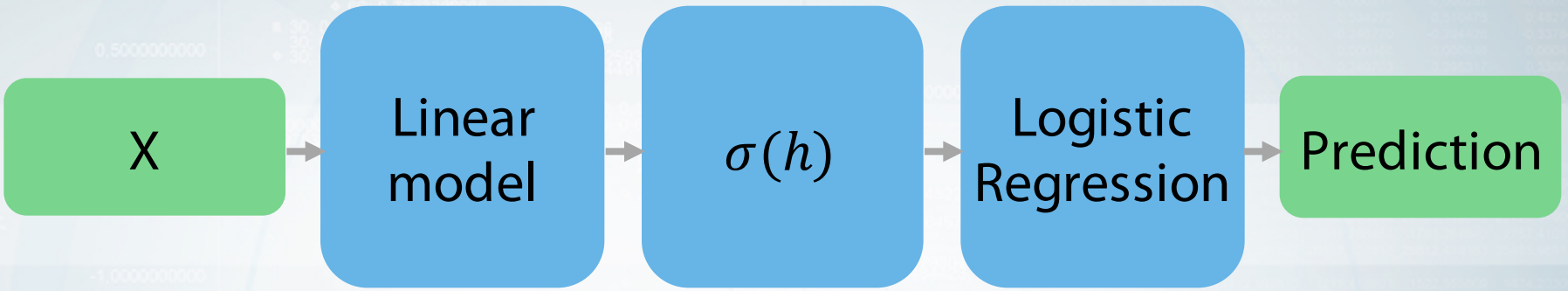


$$h_j = \sigma\left(\sum_i w_{ij}^h x_i + b_j^h\right) \qquad y_{\text{pred}} = \sigma\left(\sum_j w_j^o h_j + b^o\right)$$

$$j \in \{1,2,\ldots,n\}$$

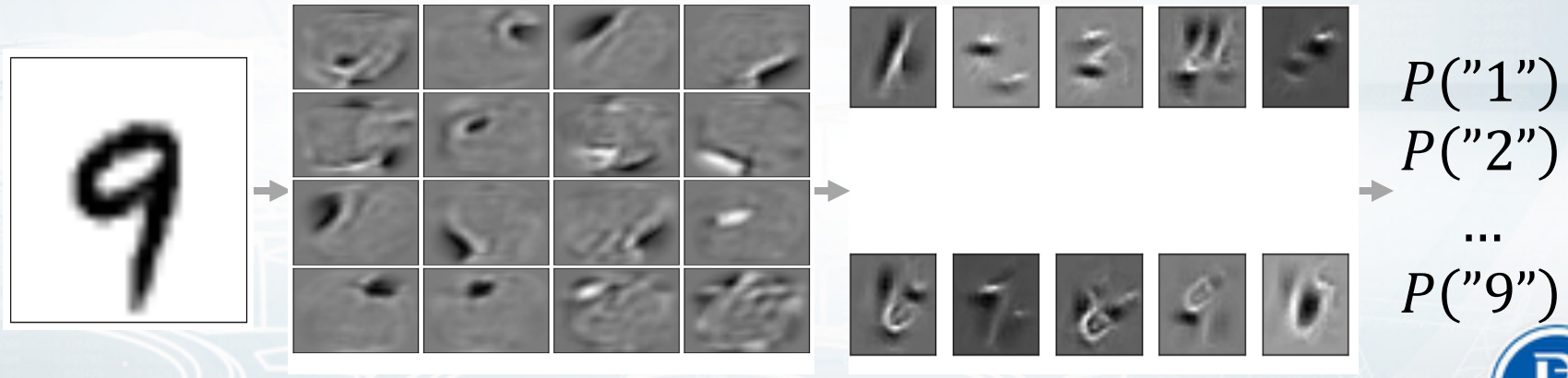
Output: $$P(y \mid x) = \sigma\left(\sum_j w_j^o \sigma\left(\sum_i w_{ij}^h x_i + b_j^h\right) + b^o\right)$$

Effect of nonlinearity



$$h_j = \sigma\left(\sum_i w_{ij}^h x_i + b_j^h\right) \qquad y_{\text{pred}} = \sigma\left(\sum_j w_j^o h_j + b^o\right)$$

$$j \in \{1,2,\ldots,n\}$$



Balakrishnan Prabhu, https://corpocrat.com/2014/10/17/machine-learning-using-restricted-boltzmann-machines/

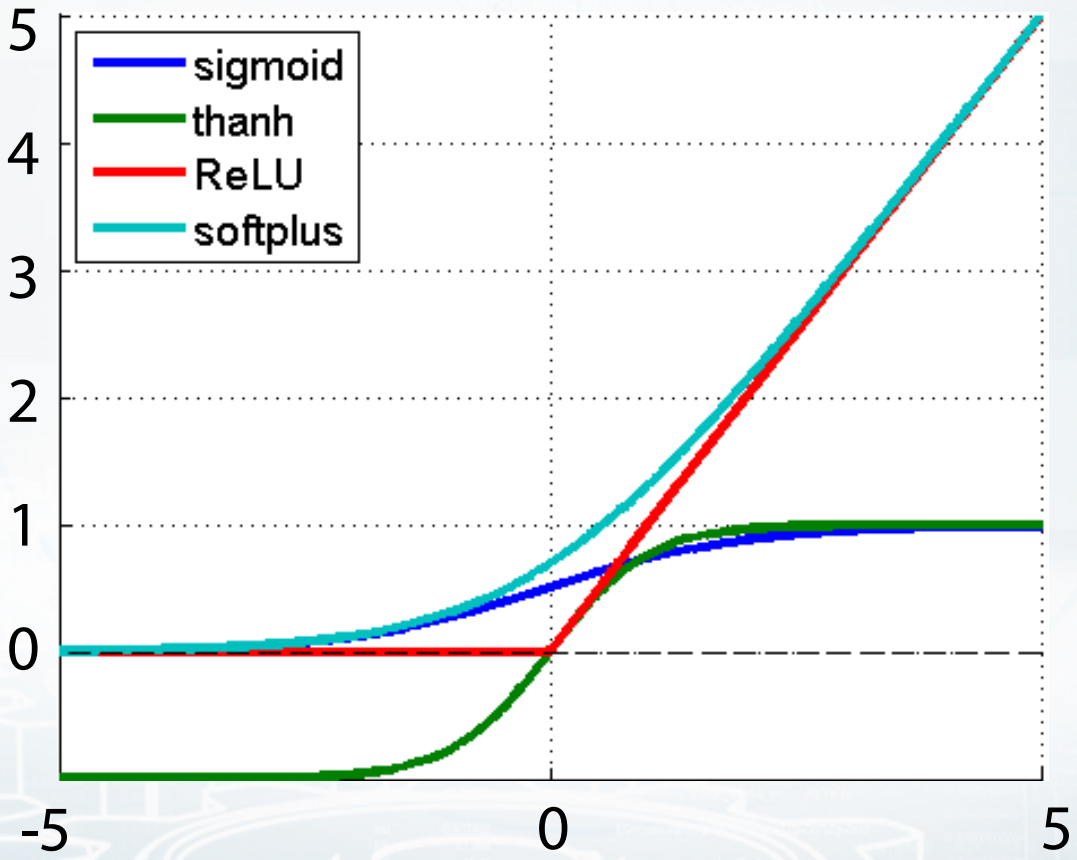
Types of nonlinearity

$$f(a) = \frac{1}{1 + e^{a}}$$

$$f(a) = \max(0, a)$$

$$f(a) = \tanh(a)$$

$$f(a) = \log(1 + e^{a})$$



Wei Di, https://imiloainf.wordpress.com/2013/11/06/rectifier-nonlinearities/

Recap and terminology

- Layer is a building block for neural network:
  - Input layer
  - Dense layer: $f(x) = Wx + b$
  - Nonlinearity layer: $f(x) = \sigma(x)$
  - A few more: we will cover later
  - Output layer

  } Hidden layers

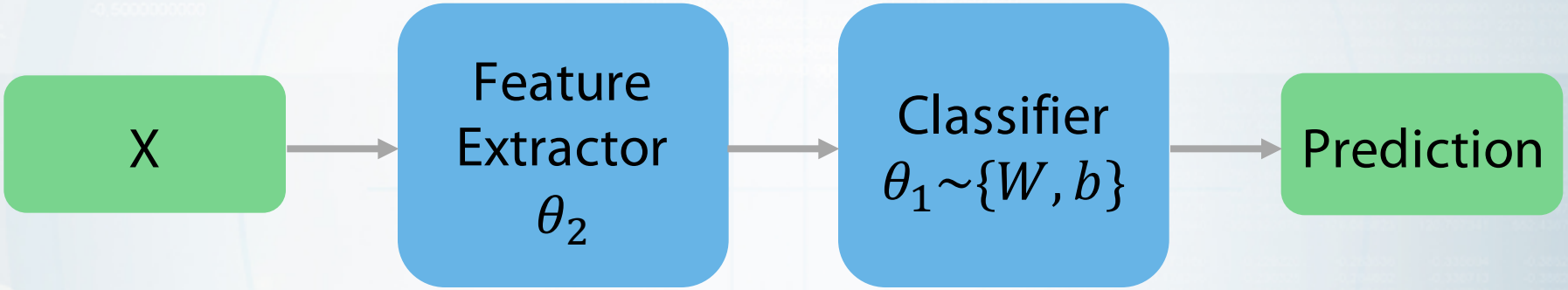
- Activation is layer output
  - i. e. some intermediate signal in the neural network

Potential caveats?

- Hardcore overfitting
- No “golden standard” for architecture
- Computationally heavy

Training a neural network

Training?



Training: $\underset{\theta_1, \theta_2}{\operatorname{argmin}} L\big(y, P(y|x)\big)$

Optimization!

Deep model is just a (composite!) function

- $f_1(f_2(f_3(x, w_3), w_2), w_1) \rightarrow loss$
- x – features vector
- $w_{1,2,3}$ – model parameters

Remember those optimization methods from the last week?
But they need gradient…

Differentiation recap

$$f : \mathbb{R} \to \mathbb{R}$$

You know what to do

Differentiation recap

$$f: \mathbb{R}^n \rightarrow \mathbb{R}$$

X is now a vector $[x_1, x_2, \ldots, x_n]$

f' is now a vector of partial derivatives $\frac{df}{dx} = \left[\frac{df}{dx_1}, \frac{df}{x_2}, \ldots, \frac{df}{x_n}\right]$

Differentiation recap

$$f: \mathbb{R}^n \rightarrow \mathbb{R}^m$$

X is a vector $[x_1, x_2, \ldots, x_n]$

f is also vector $[f_1, f_2, \ldots, f_m]$

f' is now a Jacobian matrix

$$\frac{df}{dx} = \left[\frac{df}{dx_1} \cdots \frac{df}{dx_n}\right] = \begin{bmatrix} \frac{df_1}{dx_1} & \cdots & \frac{df_1}{dx_n} \\ \vdots & \ddots & \vdots \\ \frac{df_m}{dx_1} & \cdots & \frac{df_m}{dx_n} \end{bmatrix}$$

Chain rule

$$L(x) = g\big(f(x)\big)$$

For $f, g : \mathbb{R} \to \mathbb{R}$ $\quad \dfrac{dL}{dx} = \dfrac{dg}{df} \cdot \dfrac{df}{dx}$

$$\left.\frac{dL}{dx}\right|_{x=x_0} = \left.\frac{dg}{df}\right|_{u=f(x_0)} \cdot \left.\frac{df}{dx}\right|_{x=x_0}$$

Backpropagation

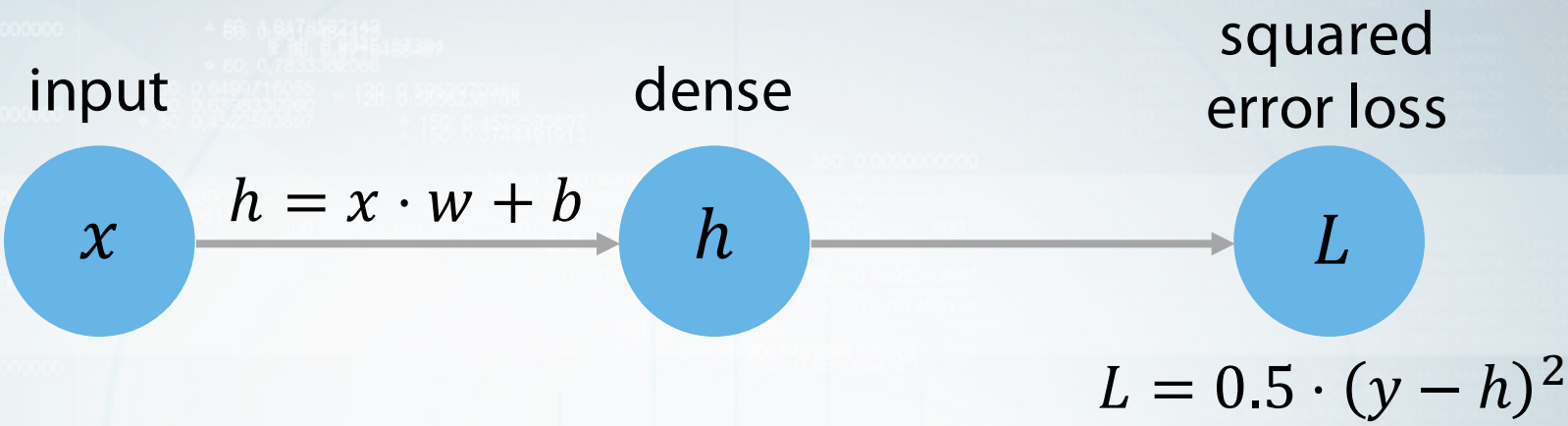
Chain rule can be evaluated numerically!

1. Compute network output and the loss value
2. Compute $\frac{\text{dLoss}}{\text{dActivation\_of\_the\_last\_layer}}$
3. For each layer, starting from the last:
    1. Compute $\frac{\text{dActivation}}{\text{dLayer\_parameters}}$, $\frac{\text{dActivation}}{\text{dLayer\_input}}$
    2. Multiply it by $\frac{\text{dLoss}}{\text{dActivation}}$, get $\frac{\text{dLoss}}{\text{...}}$
    3. Make optimization step for the parameters

Summary

- Neural network training is an optimization problem
- Commonly solved via gradient-based methods
- Gradients are computed via backpropogation

The simplest NN ever

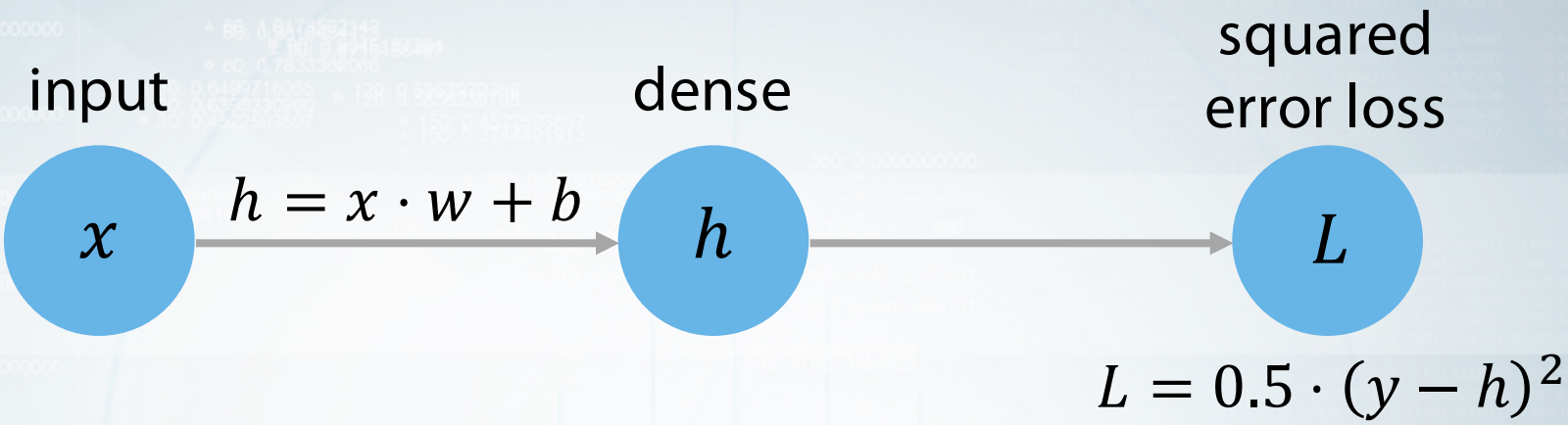


AKA
Least squares linear regression

Parameters:
Weight w, bias b

Input: x
Target: y

The simplest NN ever



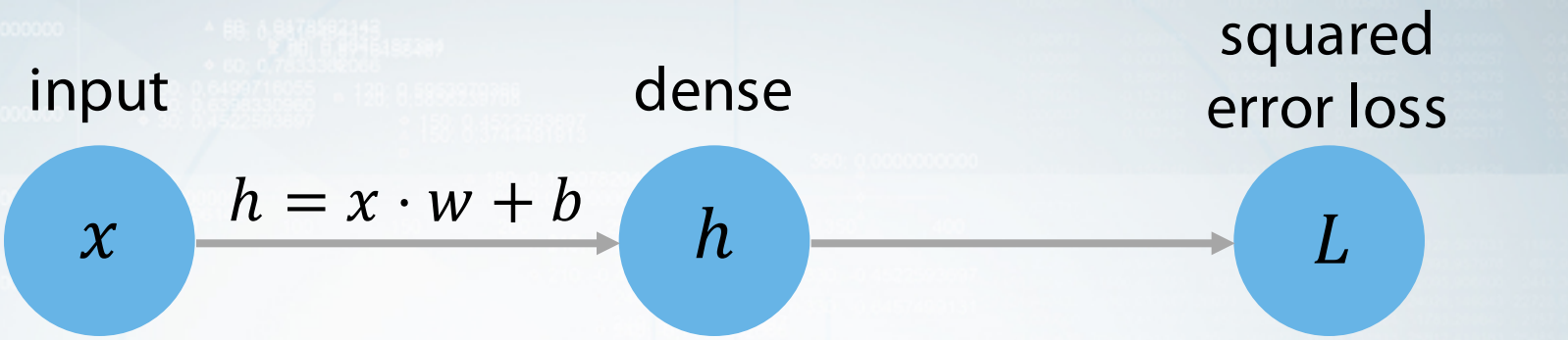
Parameters:
Weight w, bias b

Input: x
Target: y

L is just a function of parameters, features and target

$$L = f\big(y, g(x, w, b)\big)$$

The simplest NN ever



Gradient?

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial w}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial b}$$

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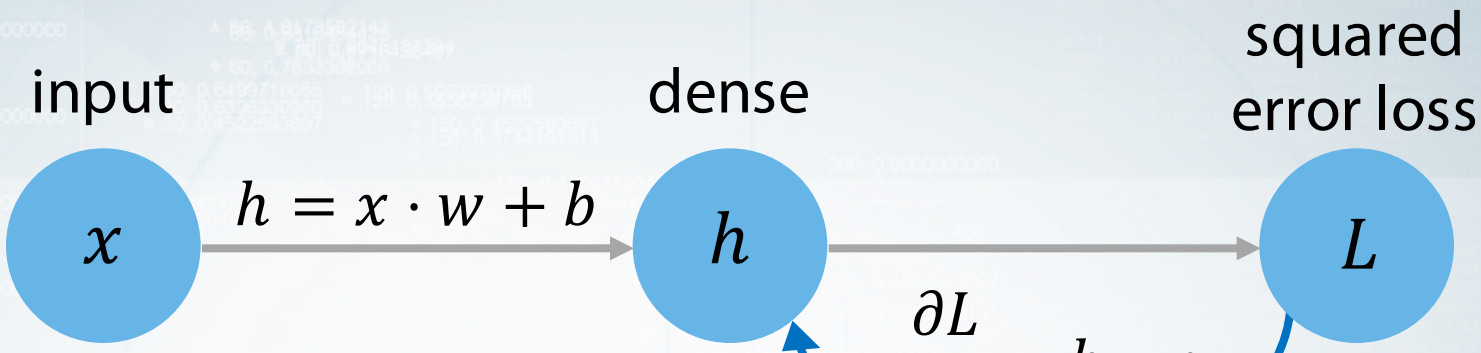
The simplest NN ever

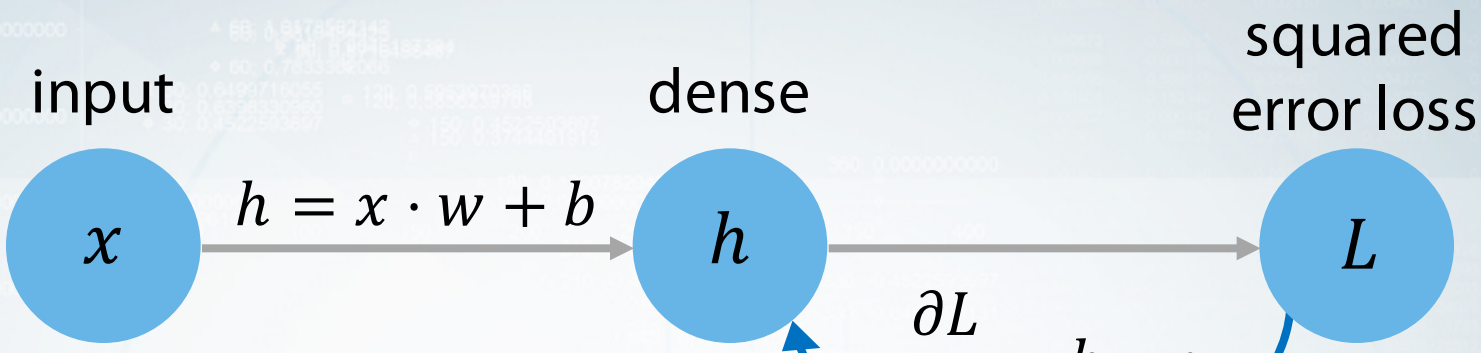


Gradient?

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial w}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial b}$$

The simplest NN ever

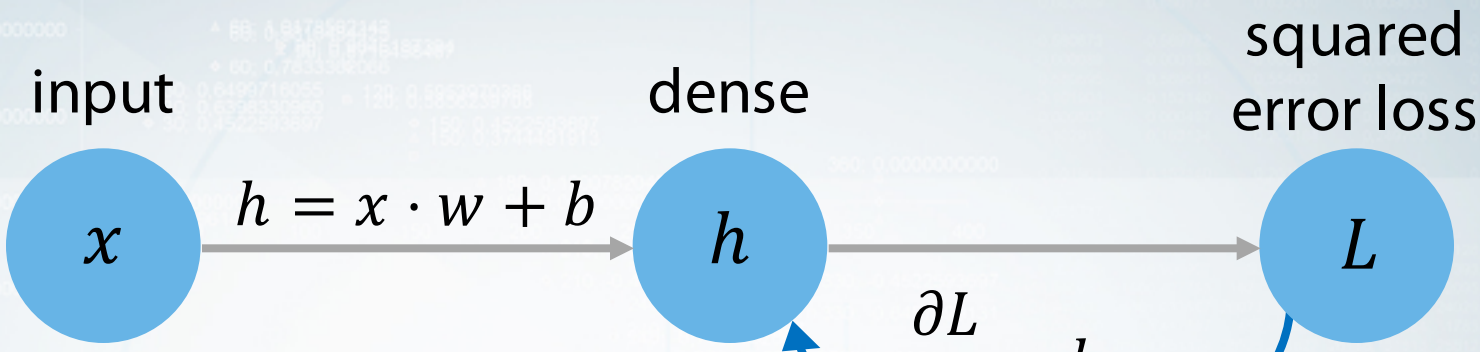


Gradient?

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial w}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial b}$$

The simplest NN ever



$$\frac{\partial h}{\partial b} = 1$$

$$\frac{\partial h}{\partial w} = x$$

$$L = 0.5 \cdot (y - h)^2$$

Let's fit

$y = 3$

$x = 1$

Initial

$w = 0.1$

$b = 1$

h	L	$\frac{\partial L}{\partial h}$	$\frac{\partial L}{\partial w}$	$\frac{\partial L}{\partial b}$	w	b
1.1	1.80					

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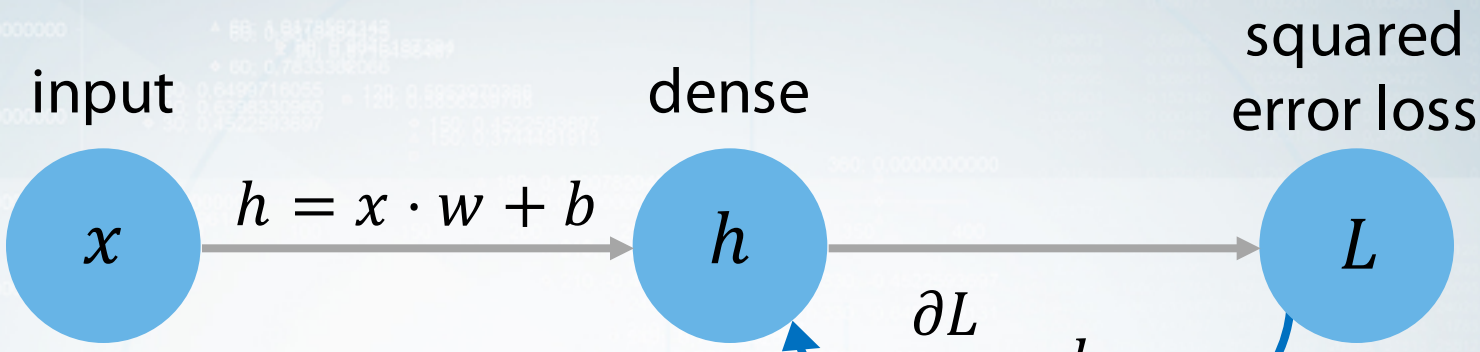
The simplest NN ever



$$\frac{\partial h}{\partial b} = 1$$

$$\frac{\partial h}{\partial w} = x$$

$$L = 0.5 \cdot (y - h)^2$$

Let's fit

$y = 3$

$x = 1$

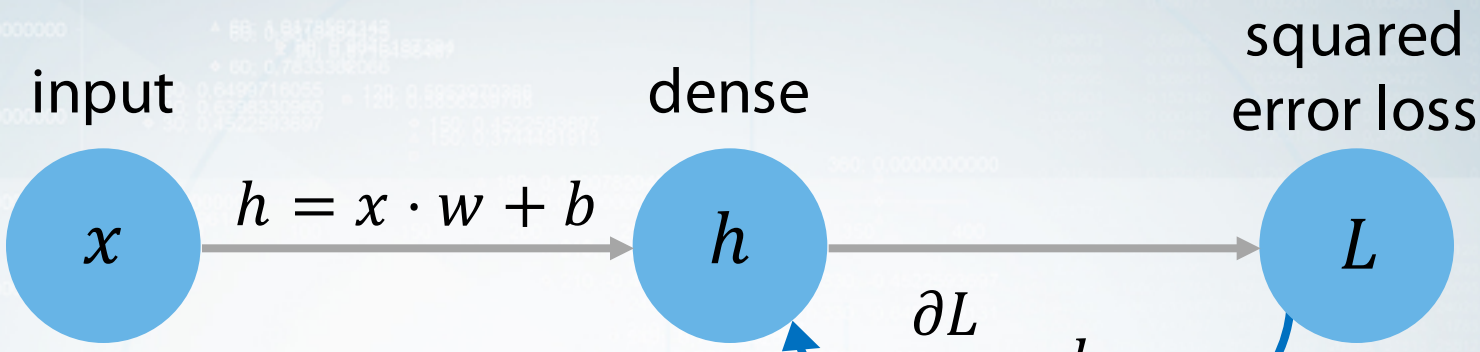
Initial

$w = 0.1$

$b = 1$

h	L	$\frac{\partial L}{\partial h}$	$\frac{\partial L}{\partial w}$	$\frac{\partial L}{\partial b}$	w	b
1.1	1.80	-1.9	-1.9	-1.9		

The simplest NN ever



Parameters update

$$w -= \eta \frac{\partial L}{\partial w}$$

$$b -= \eta \frac{\partial L}{\partial b}$$

$$\eta = 0.2$$

h	L	$\frac{\partial L}{\partial h}$	$\frac{\partial L}{\partial w}$	$\frac{\partial L}{\partial b}$	w	b
1.1	1.80	-1.9	-1.9	-1.9	0.48	1.38

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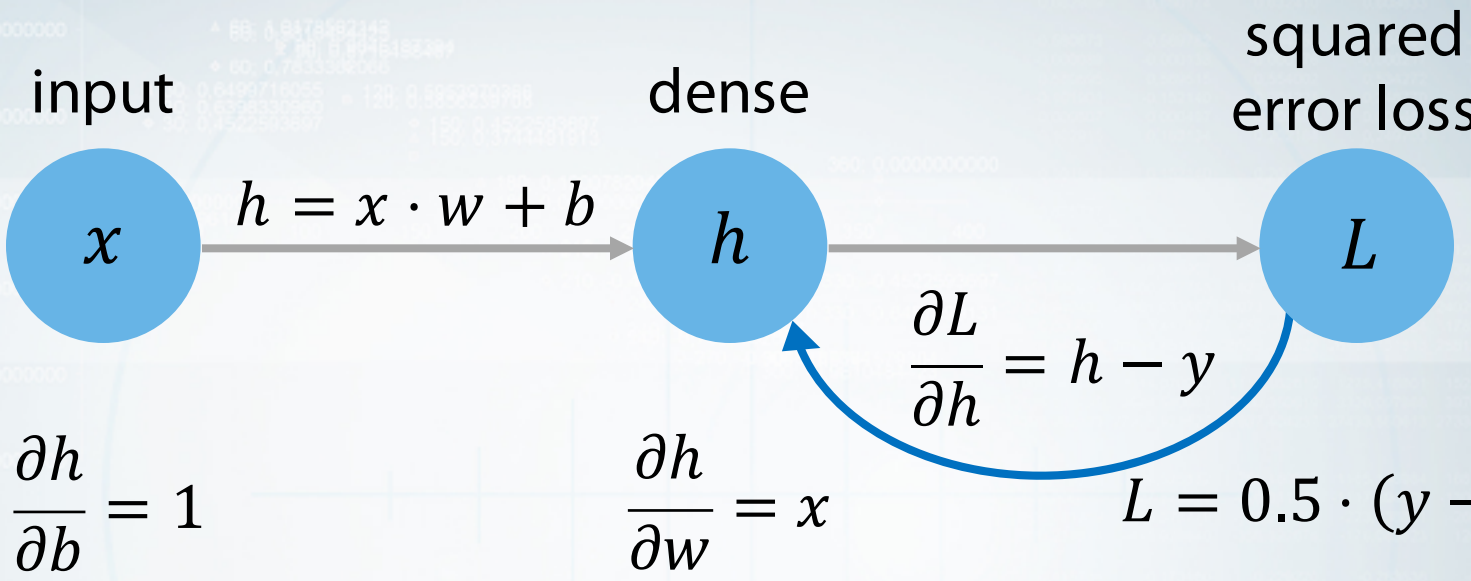
The simplest NN ever



Parameters update

$$w -= \eta \frac{\partial L}{\partial w}$$

$$b -= \eta \frac{\partial L}{\partial b}$$

$$\eta = 0.2$$

h	L	$\frac{\partial L}{\partial h}$	$\frac{\partial L}{\partial w}$	$\frac{\partial L}{\partial b}$	w	b
1.1	1.80	-1.9	-1.9	-1.9	0.48	1.38
1.86	0.65	-1.14	-1.14	-1.14	0.71	1.61
2.32	0.23	-0.68	-0.68	-0.68	0.84	1.75

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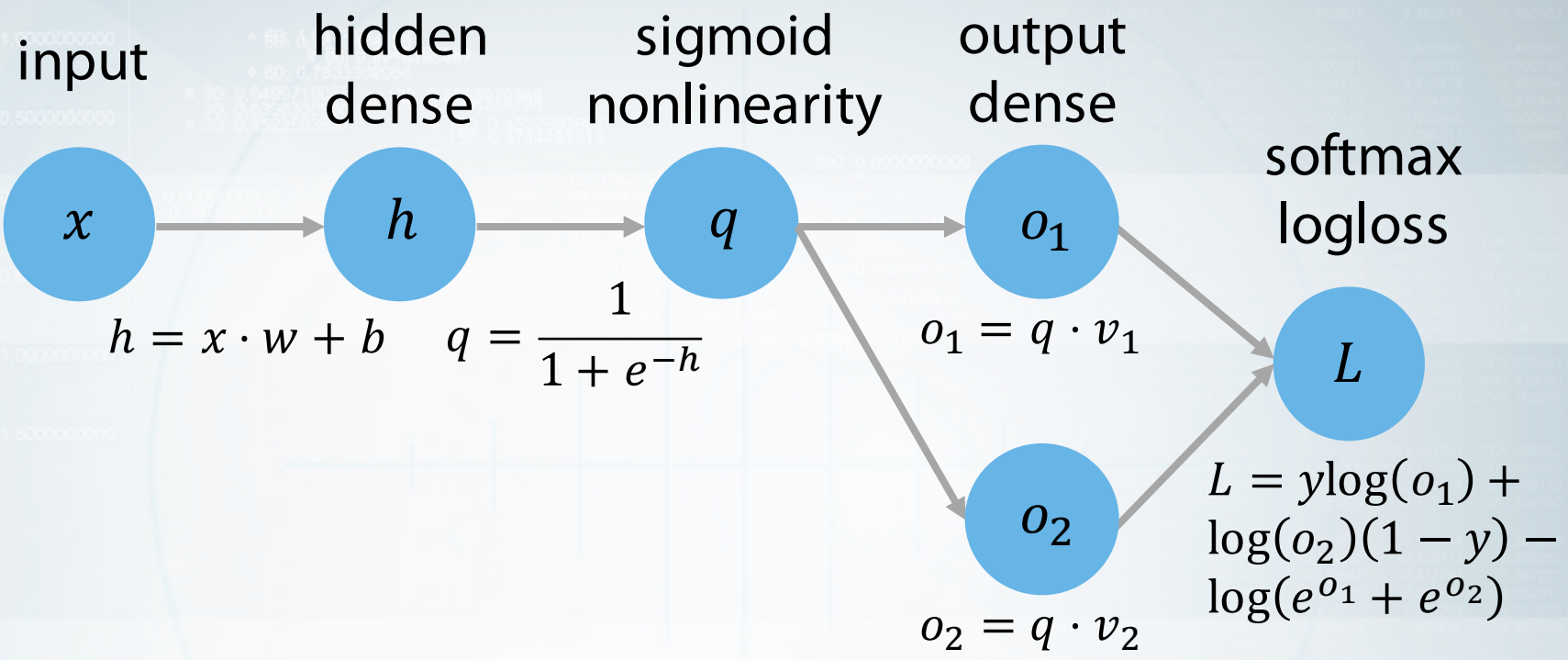
What if we go deeper?

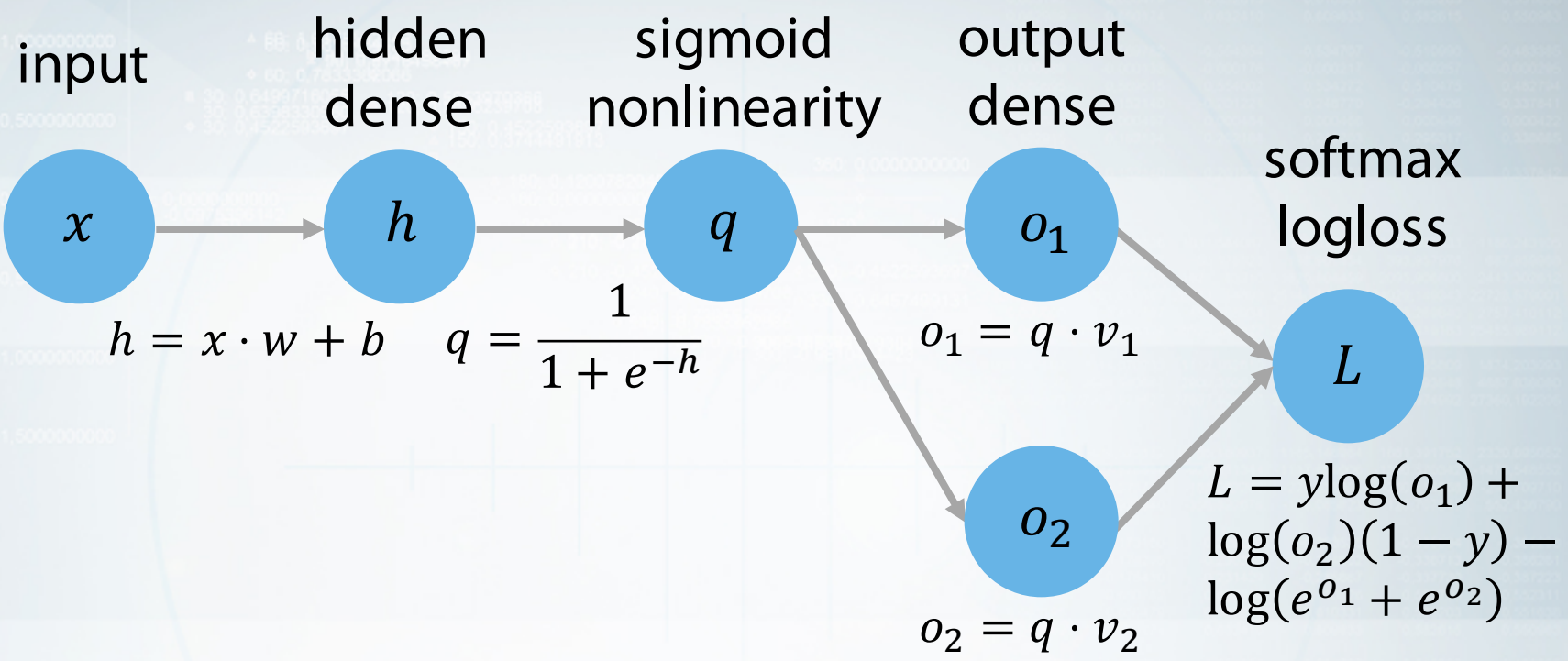


Parameters:

Weight w, bias b

Weight v_1, v_2

What if we go deeper?



Parameters:

Weight w, bias b

Weight v_1, v_2

$$\frac{dL}{do_1} = \frac{y}{o_1} - \frac{e^{o_1}}{e^{o_2} + e^{o_1}}$$

$$\frac{dL}{do_2} = \frac{1 - y}{o_2} - \frac{e^{o_2}}{e^{o_2} + e^{o_1}}$$

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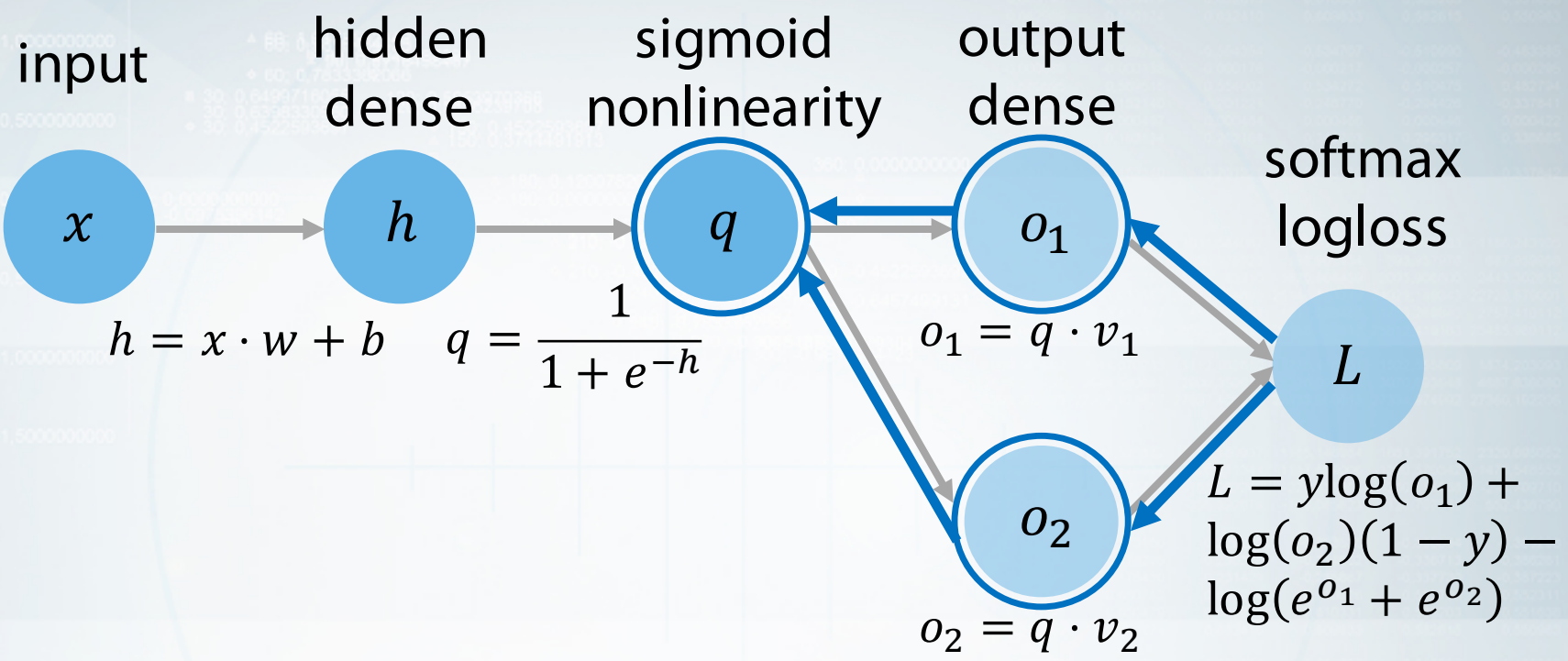
What if we go deeper?



Parameters:

Weight w, bias b

Weight v_1, v_2

$$\frac{\partial L}{\partial q} = v_1 \cdot \frac{\partial L}{\partial o_1} + v_2 \cdot \frac{\partial L}{\partial o_2}$$

Update v_1, v_2

$$\frac{\partial L}{\partial v_1} = \frac{\partial L}{\partial o_1} \cdot q \quad \frac{\partial L}{\partial v_2} = \frac{\partial L}{\partial o_2} \cdot q$$

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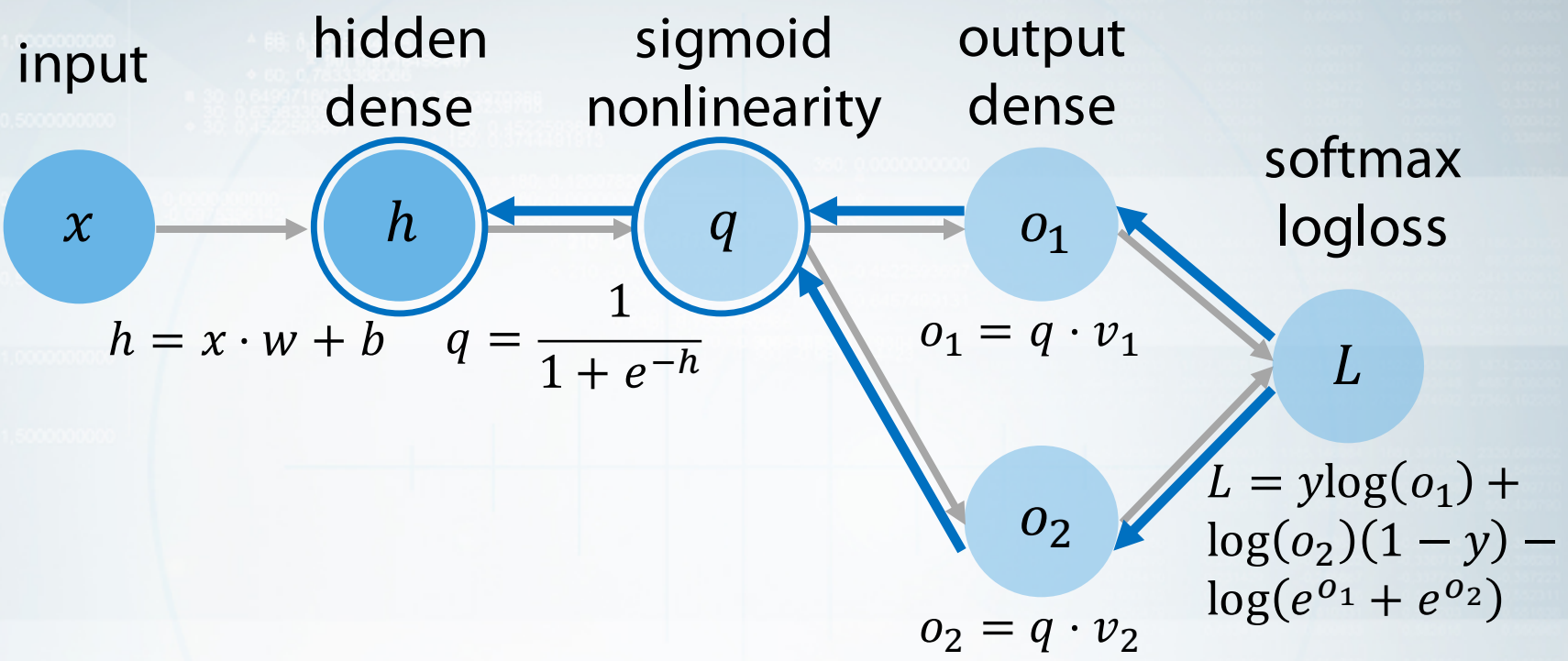
What if we go deeper?



Parameters:

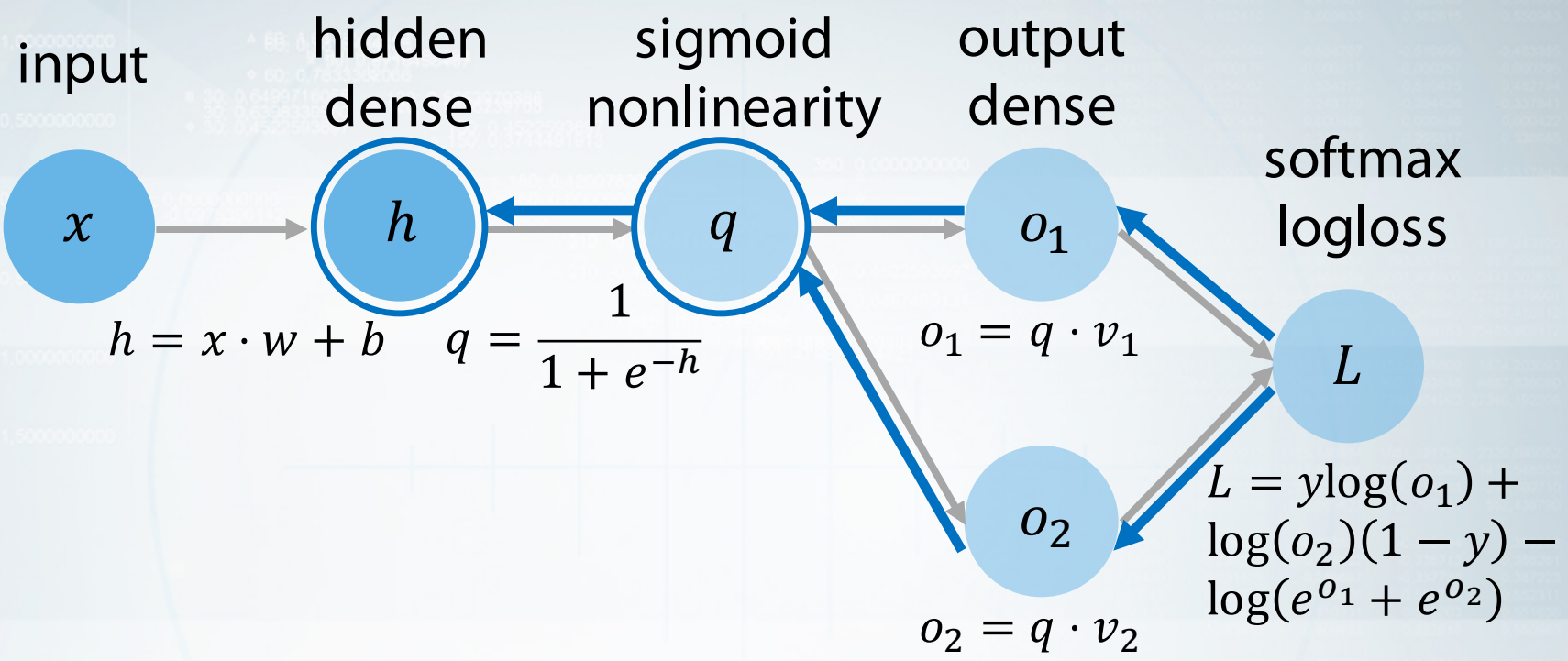
Weight w, bias b

Weight v_1, v_2

Question.

What will the derivative $\frac{\partial q}{\partial h}$ be?

What if we go deeper?



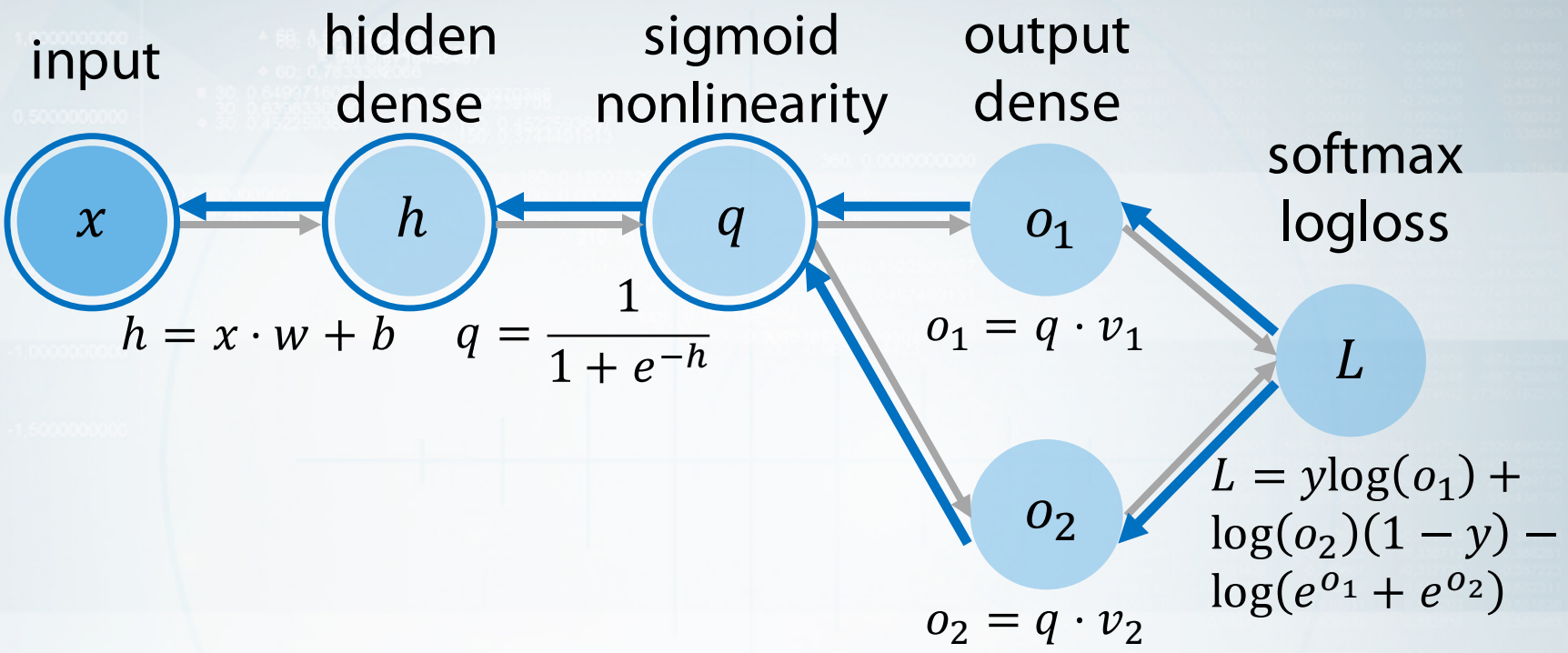
Parameters:

Weight w, bias b

Weight v_1, v_2

$$\frac{\partial L}{\partial h} = \frac{\partial L}{\partial q} \frac{e^{-q}}{(1 + e^{-q})^2}$$

What if we go deeper?



Parameters:

Weight w, bias b

Weight v_1, v_2

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial h} \cdot x$$

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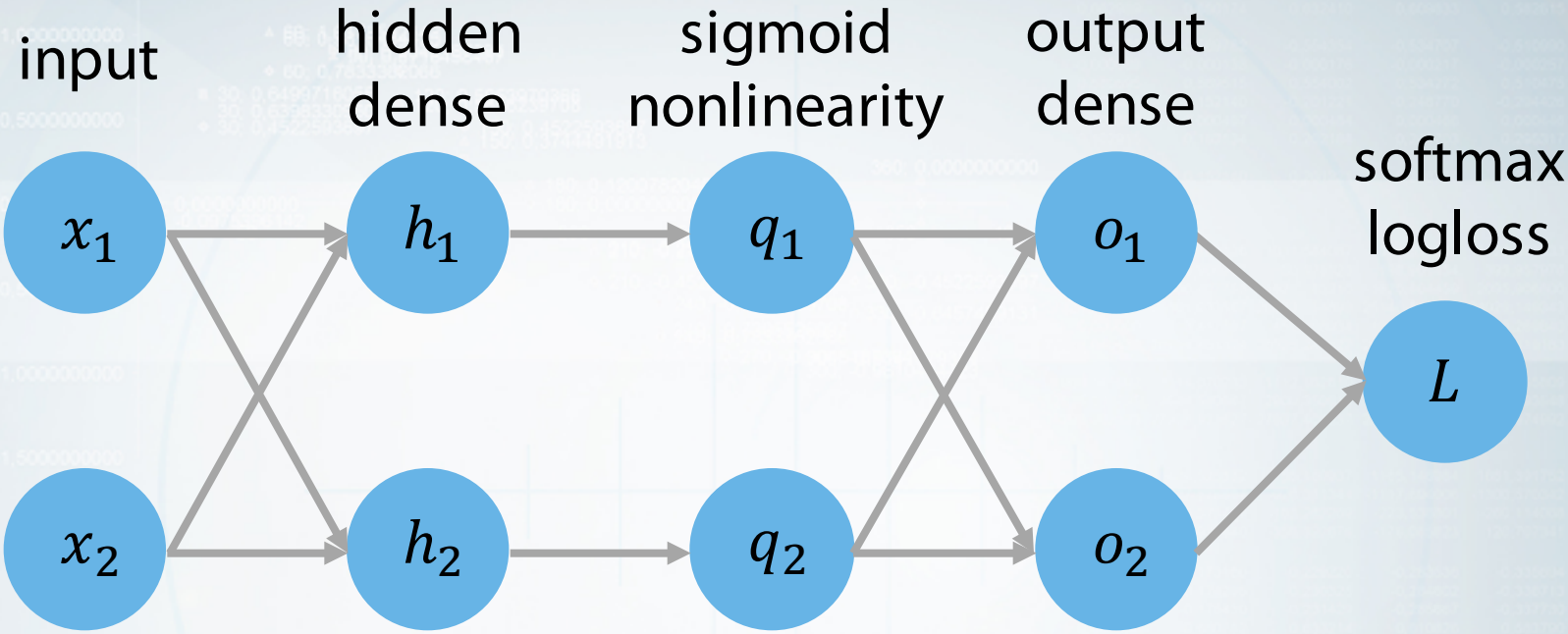
What if we go wider?



$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + b \qquad \begin{bmatrix} o_1 \\ o_2 \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \cdot \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

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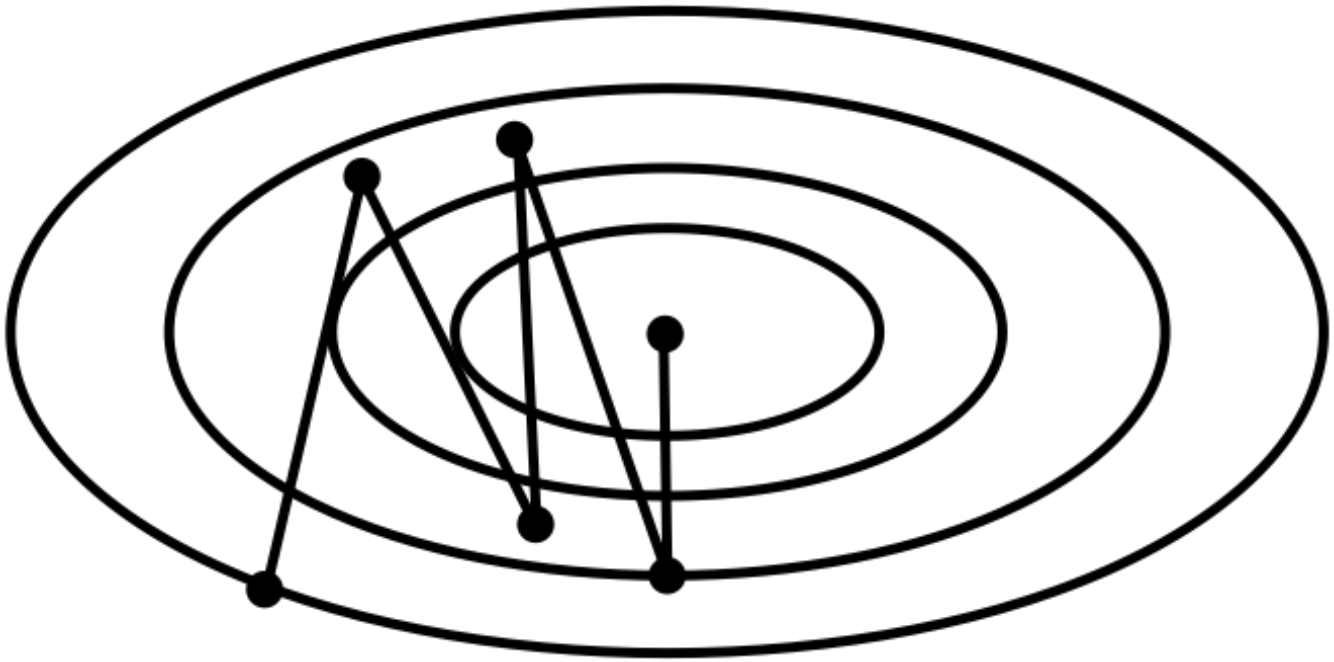
What's in it for me?

You can have any crazy layer as long as you can compute its gradient

- No need to compute the gradients by hand
- There are many frameworks for that

Gradient descent extensions

Difficult function



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Mini-batch gradient descent

w^0 — initialization

while True:

$i_1, \ldots, i_m$ = random indices between 1 and ℓ

$$g_t = \frac{1}{m}\sum_{j=1}^{m} \nabla L\left(w^{t-1}; x_{i_j}; y_{i_j}\right)$$

$$\boldsymbol{w^t = w^{t-1} - \eta_t g_t}$$

if $\|w^t - w^{t-1}\| < \epsilon$ then break

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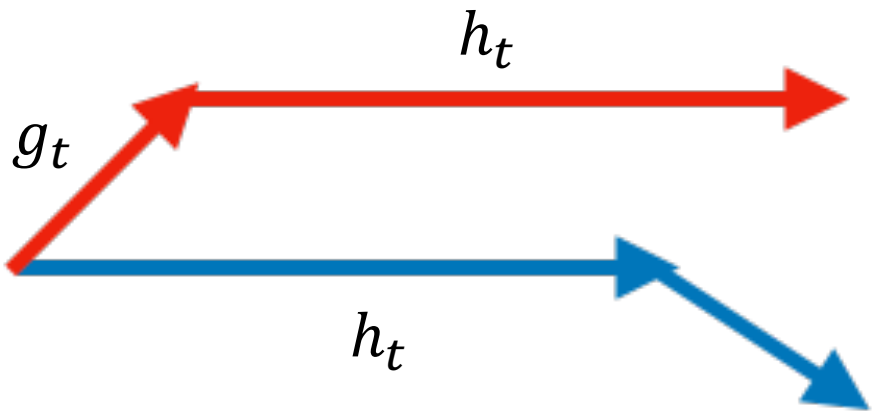
Momentum

$$h_t = \alpha h_{t-1} + \eta_t g_t$$

$$w^t = w^{t-1} - h_t$$

- Tends to move in the same direction as on previous steps
- h_t accumulates values along dimensions where gradients have the same sign
- Usually: $\alpha = 0.9$

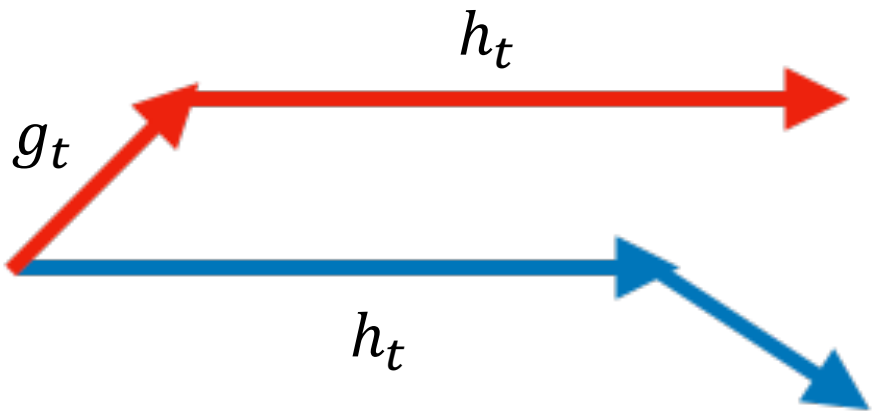
Nesterov momentum



Nesterov momentum

$$h_t = \alpha h_{t-1} + \eta_t \nabla L(w^{t-1} - \alpha h_{t-1})$$

$$w^t = w^{t-1} - h_t$$



AdaGrad

$$G_j^t = G_j^{t-1} + g_{tj}^2$$

$$w_j^t = w_j^{t-1} - \frac{\eta_t}{\sqrt{G_j^t + \epsilon}} g_{tj}$$

- g_{tj} — gradient with respect to j-th parameter
- Separate learning rates for each dimension
- Suits for sparse data
- Learning rate can be fixed: $\eta_t = 0.01$
- G_j^t always increases, leads to early stops

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RMSprop

$$G_j^t = \alpha G_j^{t-1} + (1-\alpha) g_{tj}^2$$

$$w_j^t = w_j^{t-1} - \frac{\eta_t}{\sqrt{G_j^t + \epsilon}} g_{tj}$$

- α is about 0.9
- Learning rate adapts to latest gradient steps

Adam

$$v_j^t = \frac{\beta_2 v_j^{t-1} + (1-\beta_2) g_{tj}^2}{1-\beta_2^t}$$

$$w_j^t = w_j^{t-1} - \frac{\eta_t}{\sqrt{v_j^t + \epsilon}} g_{tj}$$

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Adam

$$m_j^t = \frac{\beta_1 m_j^{t-1} + (1-\beta_1) g_{tj}}{1-\beta_1^t}$$

$$v_j^t = \frac{\beta_2 v_j^{t-1} + (1-\beta_2) g_{tj}^2}{1-\beta_2^t}$$

$$w_j^t = w_j^{t-1} - \frac{\eta_t}{\sqrt{v_j^t + \epsilon}} m_j^t$$

Combines momentum and individual learning rates

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Summary

- Momentum methods smooth gradients and speed up convergence
- Adaptive methods eliminate sensitive learning rate
- Adam combines both approaches

Lecture Summary

Neural Networks:

- approximate **any** functions
- are trained via backpropagation algorithms
- can easily overfit

Main nonlinear functions:

- ReLU and its modifications (GeLU, ELU, etc.)
- Sigmoid
- Tanh

Main Optimization algorithms:

- AdamW
- SGD