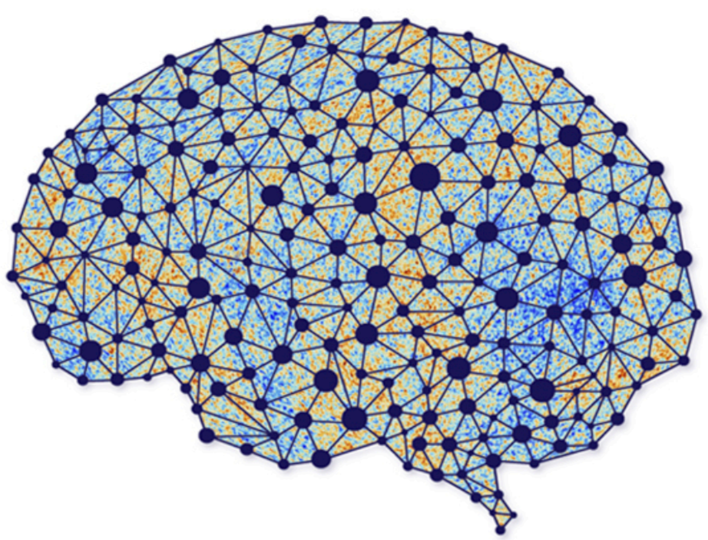
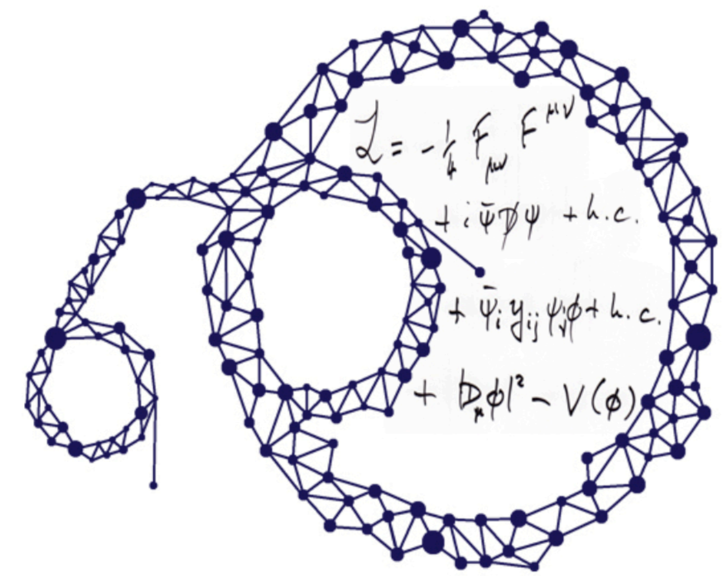
Physics 361 - Machine Learning in Physics

Lecture 4 – Basics of Machine Learning

Jan. 29th 2025



AI
∩
Universe



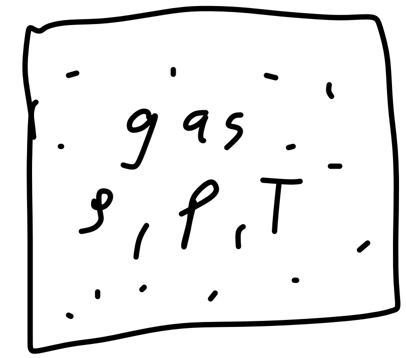
Moritz Münchmeyer

Unit 1: Background

1.4 Information theory background (cont.)

Entropy

- In statistical physics (thermodynamics) the entropy is given by



$$S = (k_B) \log \Omega$$

here we set it to 1

Ω: number of microstates (equally likely)

- We can re-write this as

$$S = -\log p \quad \text{where} \quad p = \frac{1}{\Omega}$$

is the probability of each m. state

- The general definition of entropy

Shannon entropy $$\boxed{S = -\sum_i p_i \log p_i}$$

- log here is base e $\rightarrow$ entropy is in „nats"

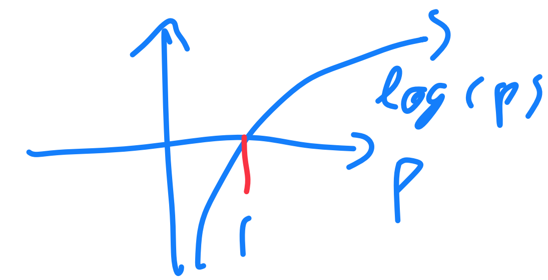
(base 2 $\rightarrow$ " in bits)

Properties of the entropy

- <u>discrete PDF</u> $$S = -\sum_i p_i \underbrace{\log(p_i)}$$

$-\log(p_i)$ is the „self-information" of event i

$$= -\mathbb{E}_{x \sim p(x)} \left[\log(p(x)) \right]$$



A unlikely event has a large self info.

self information $I(x) = -\log(p(x))$

A certain event has self inform. 0

maximum possible entropy is $S = \log(N)$

- <u>continuous PDF</u> $$S = -\int dx\, p(x) \log(p(x))$$

$$= -\mathbb{E}_{x \sim p(x)} \left[\log(p(x)) \right]$$

More uniform distributions have a higher entropy.
(spread out)

Kullback - Leibler divergence

- The relative entropy = KL divergence provides a measure of the similarity of two probab. distr. $P(x)$ and $Q(x)$:

difference of self information of sample x

$$D_{\mathrm{KL}}(P\|Q) = \mathbb{E}_{\mathrm{x}\sim P}\left[\log \frac{P(x)}{Q(x)}\right] = \mathbb{E}_{\mathrm{x}\sim P}\left[\log P(x) - \log Q(x)\right]$$

- If P and Q are the same then $D_{KL} = 0$.

  e.g in generative ML

  $P(x)$: true (unknown) PDF of the training images

  $Q(x)$: PDF of generated images

- D_{KL} is easy to evaluate by sampling (if P and Q are known).
- $D_{KL} \geq 0$

- Interpretation: If our data is described by P and we have a theory/model Q that is meant to describe the data, at what rate will collection of data inform me that theory Q differs from P.

  = KL divergence

- Minimizing the KL divergence is the same as maximizing the likelihood of the data given the model Q. We define the cross-entropy as the part of the KL divergence that depends on the parameters of Q.

  Cross entropy $H(P,Q) = -\mathbb{E}_{x \sim P(x)} \log [Q(x)]$

- The KL divergence is not a true distance metric. E.g. it is not symmetric in P, Q.

  Other alternatives: - Wasserstein distance
  - F-divergence

- Another interesting concept: mutual information

$$I(X,Y) = D_{KL}[\,p(x,y) \,||\, p(x)\,p(y)\,]$$

vanishes if X, Y are independent.

All of these information theory concepts are frequently used in machine learning.

Unit 2: Basics of Machine Learning

Sources: e.g. deeplearningbook.org

Overview

Most machine Learning algorithms have the following elements:

- dataset
  - training data
  - test data
  - validation data
- cost function / loss function / training objective
- model / architecture
- optimization procedure

We first discuss these at the example of curve fitting.
Then we train a simple neural network.

Unit 2: Machine Learning Basics

2.1 Machine Learning concepts using the example of Linear and Polynomial Regression

Linear regression

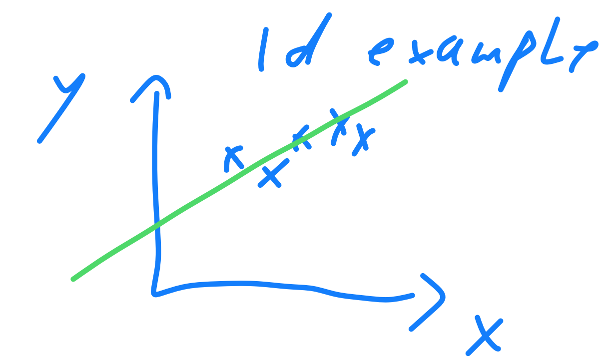
- The simplest machine learning algorithm.
- Predict 1 number from N features:

$$\hat{y} = \vec{w}^T \vec{x} + b$$

This can be re-written as

$$\hat{y} = \vec{w}^T \vec{x}$$

where we include b by adding an element 1 to x $\quad x = \begin{pmatrix} \vdots \\ 1 \end{pmatrix}$



- notation: We define the design matrix as

$$\mathbf{X} = \begin{array}{c} \\ \text{example} \end{array} \begin{array}{c} \text{features} \\ \begin{pmatrix} | & | & | & | \\ | & | & | & | \end{pmatrix} \end{array}$$

$\mathbf{X}^{\text{train}}$: training data

$\vec{y}$: training labels

vector over examples

- training set $\{\mathbf{X}^{\text{train}}, \vec{y}^{\,\text{train}}\}$

  test set $\{\mathbf{X}^{\text{test}}, \vec{y}^{\,\text{test}}\}$

- The typical cost function for such regression problems is the Mean Squared Error (MSE).

$$MSE = \frac{1}{m} \sum_i (\hat{y}_i - y_i)^2$$

prediction truth

for linear regression: $\hat{y}_i = \vec{w}^T x_i$.

- Notation: L_p norm of a vector is

$$\|\vec{x}\|_p = \left(\sum_i |x_i|^p \right)^{1/p}$$

Thus we can rewrite

$$MSE = \frac{1}{m} \| \hat{\vec{y}} - \vec{y} \|_2^2$$

- Goal is to minimize the MSE.

train to minimize MSE_{train} wrt. $\vec{w}$.

→ hope MSE_{test} will also be small.

• For linear regression we can solve for $\vec{w}$ analytically:

$$\nabla_{\boldsymbol{w}} \mathrm{MSE}_{\text{train}} = 0$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \frac{1}{m} ||\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}||_2^2 = 0$$

$$\Rightarrow \frac{1}{m} \nabla_{\boldsymbol{w}} ||\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})}||_2^2 = 0$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\right)^\top \left(\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\right) = 0$$

$$\nabla_{\boldsymbol{w}} \left(\boldsymbol{w}^\top \boldsymbol{X}^{(\text{train})\top}\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - 2\boldsymbol{w}^\top \boldsymbol{X}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})} + \boldsymbol{y}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})}\right) = 0$$

$$\Rightarrow 2\boldsymbol{X}^{(\text{train})\top}\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - 2\boldsymbol{X}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})} = 0$$

$$\Rightarrow \boxed{\boldsymbol{w} = \left(\boldsymbol{X}^{(\text{train})\top}\boldsymbol{X}^{(\text{train})}\right)^{-1}\boldsymbol{X}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})}}$$

we need matrix multiplication and inversion.

deeplearningbook.org

Background on matrix calculus

(required to understand the last slide, but not often used in this course)

derivative of quadratic forms:

1. For a symmetric matrix A:

$$\nabla_w (w^T A w) = 2Aw.$$

2. For a general (not necessarily symmetric) matrix A:

$$\nabla_w (w^T A w) = (A + A^T)w.$$

3. Gradient with respect to w^T:

$$\nabla_{w^T} (w^T A w) = w^T (A + A^T).$$

derivatives of inner products

- If $f(w) = b^T w$ for a vector b, then:

$$\nabla_w (b^T w) = b$$

- If $f(w) = w^T b$, then

$$\nabla_w (w^T b) = b$$

Properties of Transposition

- $(AB)^T = B^T A^T$
- $(A^T)^T = A$
- If A is square and invertible, then $(A^{-1})^T = (A^T)^{-1}$.

since bilinear forms are scalars we have:

$$w^T A b = (w^T A b)^T$$

much more about this:

Reference: "Matrix Cookbook" https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

Linear regression (cont'd)

Very simple ML model:

$$\hat{y} = \vec{w}^T \vec{x}$$

$\vec{x}$: input

$\vec{y}$: output

training data:

$$X^{train} = \overbrace{\left(\qquad\qquad\right)}^{\text{features}} \left.\vphantom{\Bigg(}\right\} \text{examples}$$

$$\vec{y}^{\,train} = \text{desired output} = \text{label}$$

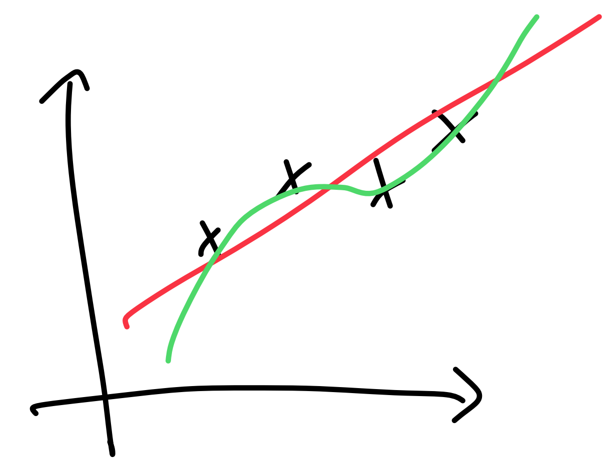
Loss function:

$$MSE = \frac{1}{m} \| \underbrace{\hat{\vec{y}}}_{\text{estimate}} - \underbrace{\vec{y}}_{\text{training "label"}} \|_2^2$$

Can be minimized w.r.t. to $\vec{w}$:

$$\vec{w} = \left(X^{train\,T} X^{train} \right)^{-1} X^{train\,T} \vec{y}^{\,train}$$

Polynomial regression



- In polynomial regression we fit a higher order polynomial.

  E.g. 2nd order pol. $\hat{y} = b + w_1 x + w_2 x^2$

  General: $\hat{y} = b + \sum_{i=1}^{N} w_i x^i$

- This model can be solved for $\vec{w}$ with the same equations as linear regression because it is still linear in the parameters w_i.

Capacity, Overfitting, Underfitting

- How well does a model trained/fitted to the training data work on novel data.
  $\Rightarrow$ Generalization error

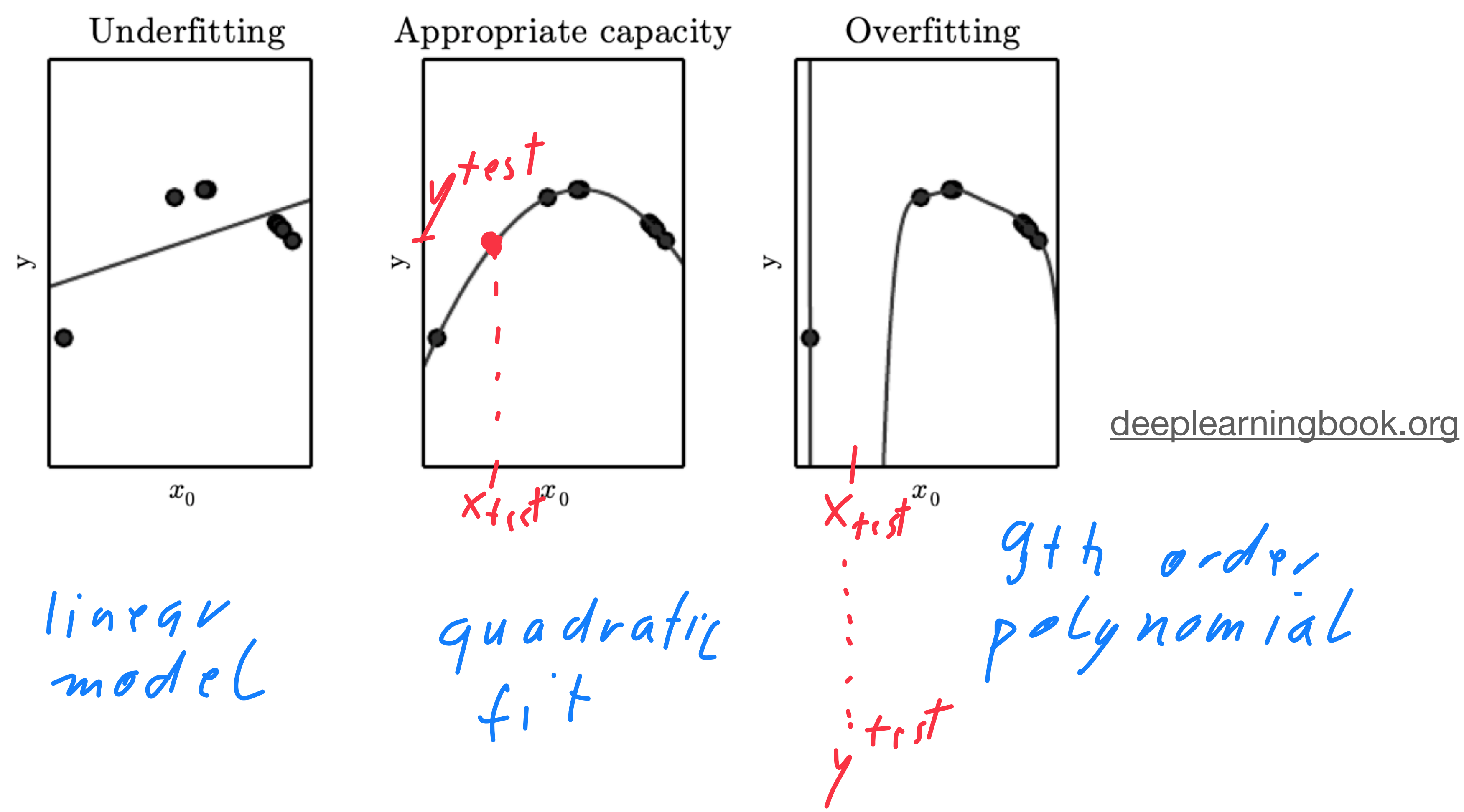
- We usually assume that training data and test data are drawn from the same distribution. „i.i.d." data: independent identically distributed

- Generalization is closely related to overfitting and underfitting.

  underfit: training error is large

  overfit: training error is small but test error is large.

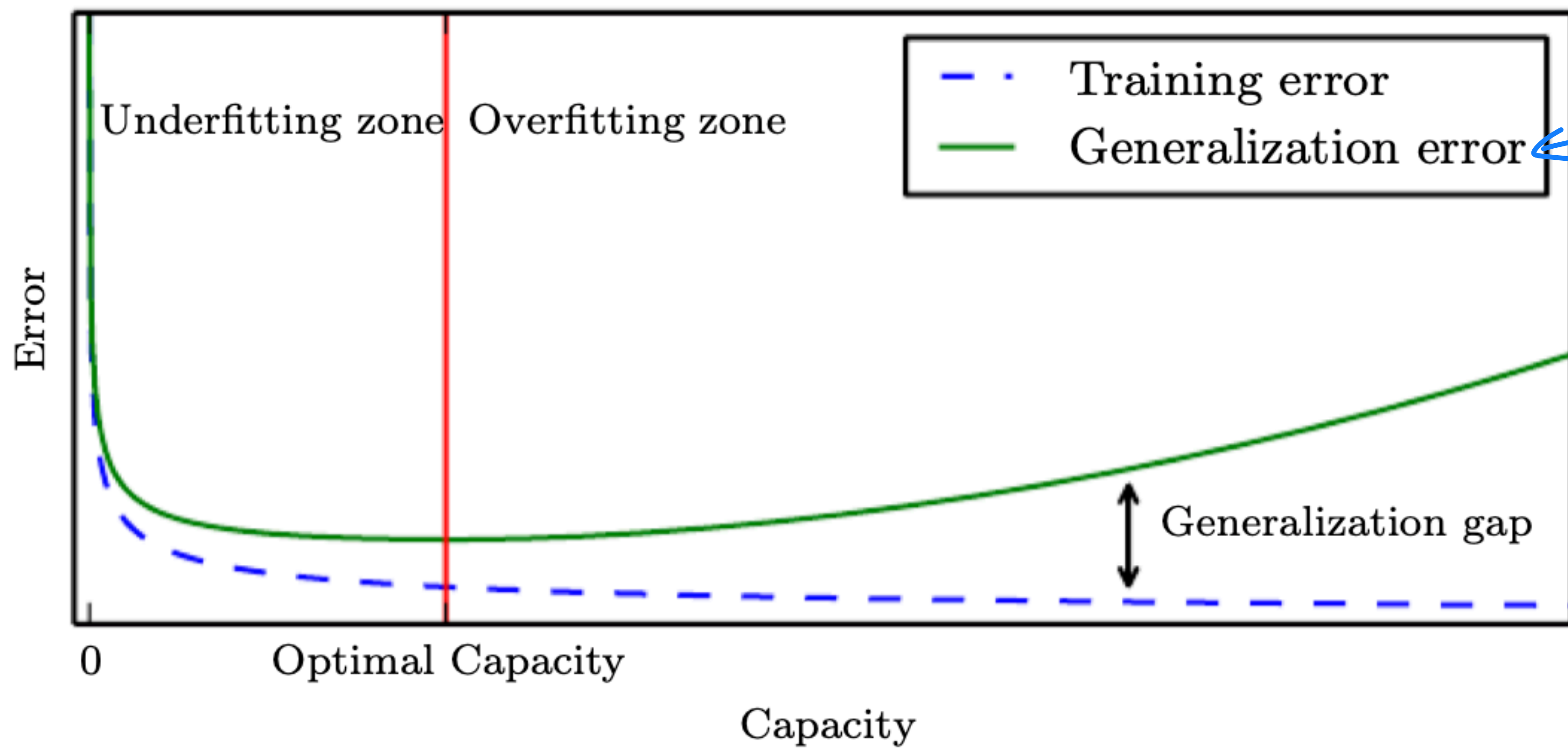
Example of polynomial regression



- The space of functions that the model can represent is called the capacity.
- Occam's razor: chose the simplest „that fits"
- Lower capacity → tends to generalize better
  Higher capacity → reduces training error.

⇒ Need to optimize the capacity or „regularize."

Typical behavior of error vs capacity (after training out the model)



error on the test data set

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We could e.g. train models with various orders of polynomials (or neural network parameter numbers).

Usually this is not the main approach. Instead we use „regularization" to avoid overfitting.

Regularization

- Idea: Keep the model capacity fix, but encourage simpler solutions.

- Common method: weight decay

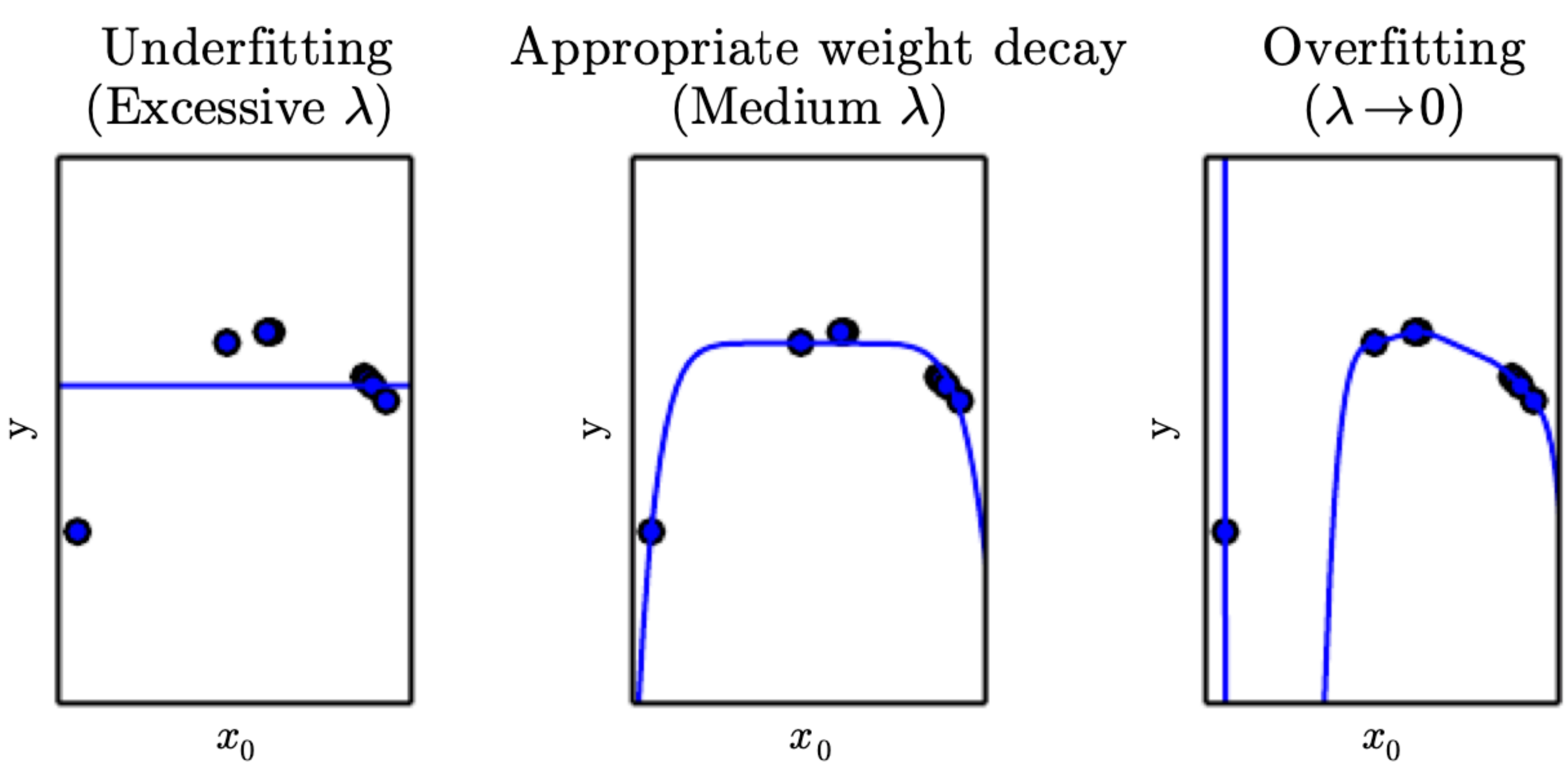
New loss to minimize $J(\vec{w}) = MSE_{train} + \lambda \underbrace{\vec{w}^T \vec{w}}$

parameter to chose "lambda"

L-2 norm

L-2 regularization

This discourages large weights



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L-2 regularization is one of several popular methods of regularization

$\boxed{\text{Regularization: any method meant to prevent overfitting without changing the model capacity.}}$

Two other popular methods which we discuss later:

- drop-out
- early stopping.

Hyperparameters

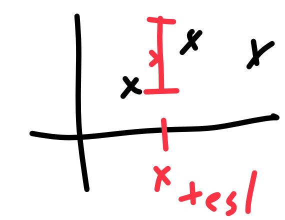
- Hyperparameters are parameters that are NOT part of the fitting/optimization procedure.

- Examples:
  - model architecture
    e.g. - maximum order of polynomials
    - depth of a neural network
  - Learning parameters
    e.g. learning rate
  - Regularization parameters e.g. λ

- To chose the best hyperparameters one often splits off a validation data set from the training data (~20% thereof).

Relation of MSE and maximum Likelihood

- In Linear regression we were Learning y from x.
  Instead now we want to Learn $p(y|x)$.
  $\Rightarrow$ we get an error bar.



- If we assume that the error is Gaussian we want to Learn:

$$p(y|x) = \mathcal{N}(y;\ \underbrace{\hat{y}(\vec{x},\vec{w})}_{\text{mean of prediction}},\ \underbrace{\sigma^2}_{\text{width of prediction error.}})$$

- The Loss is now the Likelihood of the training data:

plug in

$$\mathcal{L}(\theta) = \sum_{i=1}^{m} \log p(y^{(i)} \mid x^{(i)}; \theta)$$

model parameters, here $\vec{\theta} = \vec{w}$ in Linear regression.

$$= -m \log \sigma - \frac{m}{2} \log(2\pi) - \boxed{\sum_{i=1}^{m} \frac{|\hat{y}^{(i)}_{(\theta)} - y^{(i)}|^2}{\sigma^2}}$$

MSE Loss

- We want to maximize this with respect to θ.
  Maximize $\mathcal{L}$ is the same as minimizing MSE.

Unit 2: Machine Learning Basics

2.2 Neural Network Basics (Supervised Learning)

Supervised machine Learning

We want to Learn a complicated non-linear function to map input $\vec{x}$ to output $\vec{y}$.

$$\vec{x} \longrightarrow \boxed{f_\theta(\vec{x})} \longrightarrow \vec{y}$$

e.g. neural network

θ: model parameters = weights

We want to find the model parameters by minimizing some Loss function on our training data.

E.g.

$$L^{MSE}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left(y_i - f_\theta(\vec{x}_i) \right)^2$$

A very simple neural network

- We need some way to specify the function $f_\theta(\vec{x})$. It turns out that a very simple „architecture" works very well in practice:

  Linear transformations combined with element-wise non-linearities

- A linear transformation / linear layer* is given by $\vec{y} = \vec{f}(\vec{x}) = W\vec{x} + \vec{b}$

  $\vec{x}$: N_{dim}

  $\vec{y}$: M_{dim}

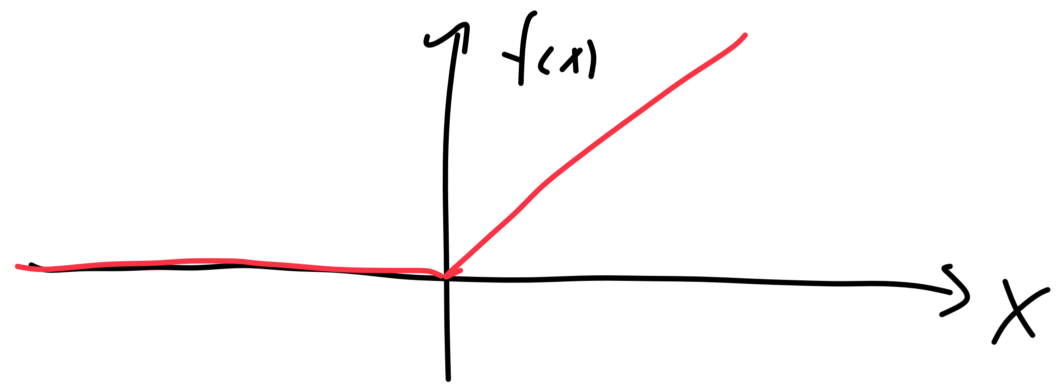
  W: matrix of weights

  $\vec{b}$: bias

- The most common non-linearity / activation function is the ReLU „rectified linear unit"

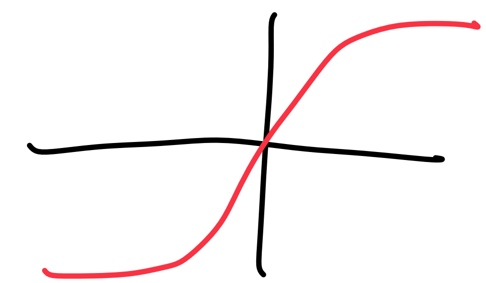
* fully connected linear layer

- ReLU is a 1-dimensional function



Piecewise linear function.

Alternatives: tanh, sigmoid



- A multilayer perceptron (MLP) is a „deep neural network" made out of a stack of the 2 building blocks.

$\vec{x} \longrightarrow \boxed{\text{Linear}} \longrightarrow \boxed{\text{reLU}} \longrightarrow \boxed{\text{Linear}} \longrightarrow \boxed{\text{reLU}} \text{ — , } \dots \longrightarrow \vec{y}$

The combination of ReLU and Linear Layer can be written as

$$f^i(x) = \underbrace{\max}_{\text{ReLU}}(0, W^i_j x^j + b^i)$$

component notation

next Layer uses $f(x)$ as x input.

If we stack these layers:

$$\max\left(0, W^i_{n,j} \max\left(0, W^j_{n-1,k} \max\left(0, \cdots\right) + b^j_{n-1}\right) + b^i_n\right)$$

Now we have a function that we can „fit" to the training data.

Loss for classification

For classification we want the NN output to be the probabilities of the various classes.

$$\vec{x} \longrightarrow \boxed{\text{MLP}} \longrightarrow y_j \xrightarrow{\text{softmax}} P_j(\vec{x})$$

e.g. image

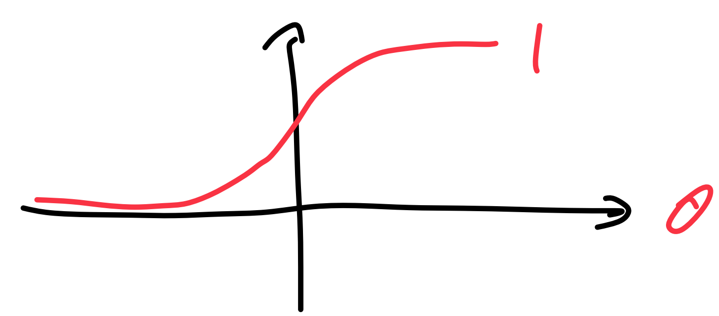
„logits" (y_j)

probability for $\vec{x}$ to be in class j. ($P_j(\vec{x})$)

A probability distribution need to have only positive probabilities and they must sum to 1.

To achive this we need the softmax function

$$P_j(y_j) = \frac{e^{y_j}}{\sum_i e^{y_i}}$$



The typical loss function for classification is the negative log likelihood = cross-entropy:

predicted by NN

$$L(\theta) = -\sum_{i=1}^{N_{examples}} \sum_{j=1}^{N_{classes}} y_j^i \log P_j(\vec{x}_i)$$

parameters of NN: W, b

$$y^i = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

one-hot vector which is 1 for the right class.

Course logistics

- **Reading for this lecture:**
  - **For example:** Deeplearningbook.org chapter 5.
- **Problem set**: First problem due Sunday night.