INTRODUCTION TO DEEP LEARNING

Course number: 00240332

Lecture 2: Math and Machine Learning Basics

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Outline

I. Math basics
II. Machine learning basics
III. Summary

Math objects

But I sometimes may not follow these conventions

- Scalar
  - A single number, often denoted by a lower case letter without boldface, e.g., a, b, x
- Vector
  - An array of numbers, often denoted by a lowercase letter with boldface, e.g., $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{x}$

$$\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

- Matrix
  - A 2D array of numbers, often denoted by an uppercase letter with boldface, e.g., $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{X}$

$$\boldsymbol{A} = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix}$$

- Tensor
  - An n-D array of numbers, often denoted like this: e.g., $\mathbf{A}, \mathbf{B}, \mathbf{X}$

$$\mathbf{A} = \left(\begin{pmatrix} A_{1,1,1} & A_{1,2,1} \\ A_{2,1,1} & A_{2,2,1} \end{pmatrix}, \begin{pmatrix} A_{1,1,2} & A_{1,2,2} \\ A_{2,1,2} & A_{2,2,2} \end{pmatrix} \right)$$

Simple operations

- Matrix transpose: $\boldsymbol{A}^\top$

$$\boldsymbol{A} = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \qquad \boldsymbol{A}^\top = \begin{pmatrix} A_{1,1} & A_{2,1} \\ A_{1,2} & A_{2,2} \end{pmatrix}$$

- A vector can be viewed as a special matrix

$$\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \qquad \boldsymbol{a}^\top = (a_1, a_2, a_3)$$

- Matrix product: if $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{B} \in \mathbb{R}^{n \times p}$, then $\boldsymbol{C} = \boldsymbol{AB}$ with shape $m \times p$ and $C_{i,j} = \sum_k A_{i,k} B_{k,j}$
- Elementwise product (Hadamard product): $\boldsymbol{C} = \boldsymbol{A} \odot \boldsymbol{B}$ where the 3 matrices are of the same shape and $C_{i,j} = A_{i,j} B_{i,j}$

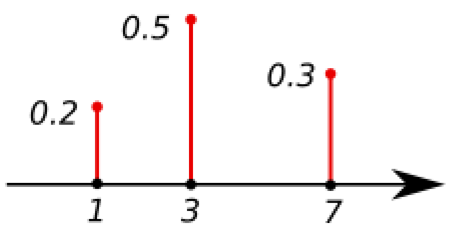
Random variable

- A random variable is a variable that can take on different values randomly
  - Denote the random variable by x and its two possible values by x_1 and x_2
  - For vectors, we write the random variable as $\mathbf{x}$ and one of its values as $\boldsymbol{x}$
  - Discrete versus continuous

Probability distribution

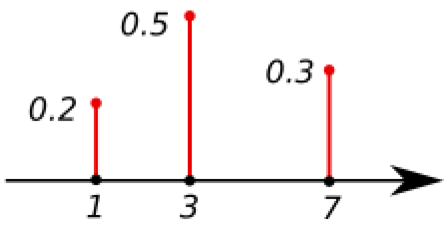
A probability distribution is a distribution of how likely a random variable or a set of random variables is to take on each of its possible states

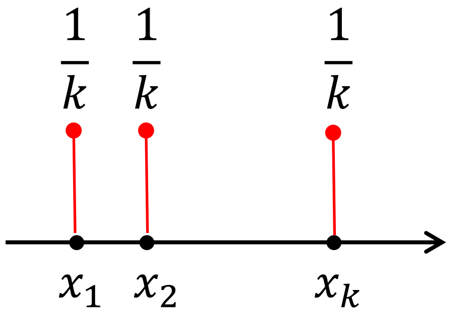
- A probability distribution over discrete variables may be described using a probability mass function (PMF)
  - The prob that $\mathrm{x} = x$ is denoted as $P(x)$ or $P(\mathrm{x} = x)$
  - $\mathrm{x} \sim P(x)$ specify which distribution x follows
- Joint probability
  - $P(\mathrm{x} = x, \mathrm{y} = y)$ or $P(x, y)$ denotes the prob that $\mathrm{x} = x$ and $\mathrm{y} = y$ simultaneously



Probability mass function

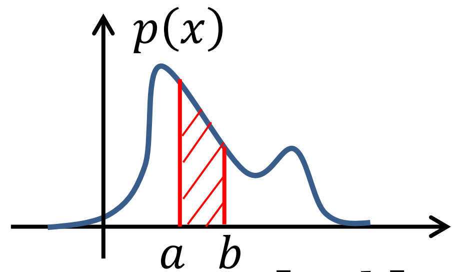
- To be a PMF of a random variable x, a function P must satisfy:
  - The domain of P must be the set of all possible states of x
  - $\forall x \in \mathrm{x}, 0 \leq P(x) \leq 1$
  - $\sum_{x \in \mathrm{x}} P(x) = 1$
- Uniform distribution
  - Consider a single discrete random variable x with k different states
  - $P(\mathrm{x} = x_i) = \frac{1}{k}, \forall\, i$





Probability density function

- A probability distribution over continuous variables may be described using a probability density function (PDF)
- To be a PDF, a function p must satisfy the following properties
  - The domain of p must be the set of all possible states of x
  - $\forall x \in \mathrm{x}, p(x) \geq 0$
  - $\int p(x)dx = 1$



Can $p(x) > 1$?

- The prob that x lies in the interval $[a, b]$ is given by $\int_a^b p(x)dx$
- Note $p(x)$ does not give the prob of a specific state directly

Typical prob distributions

- Bernoulli distribution: over a single binary random variable

$$P(\mathrm{x}=1)=\phi, P(\mathrm{x}=0)=1-\phi$$
$$P(\mathrm{x}=x)=\phi^x(1-\phi)^{1-x}$$
$$\mathbb{E}_{\mathrm{x}}[\mathrm{x}]=\phi, \mathrm{Var}(\mathrm{x})=\phi(1-\phi)$$

- Multinoulli or categorical distribution: over a single discrete variable with k different states where k is finite

$$P(\mathrm{x}=i|\boldsymbol{p})=p_i$$

where $\boldsymbol{p}\in[0,1]^k$ and $\sum_{i=1}^{k} p_i=1$

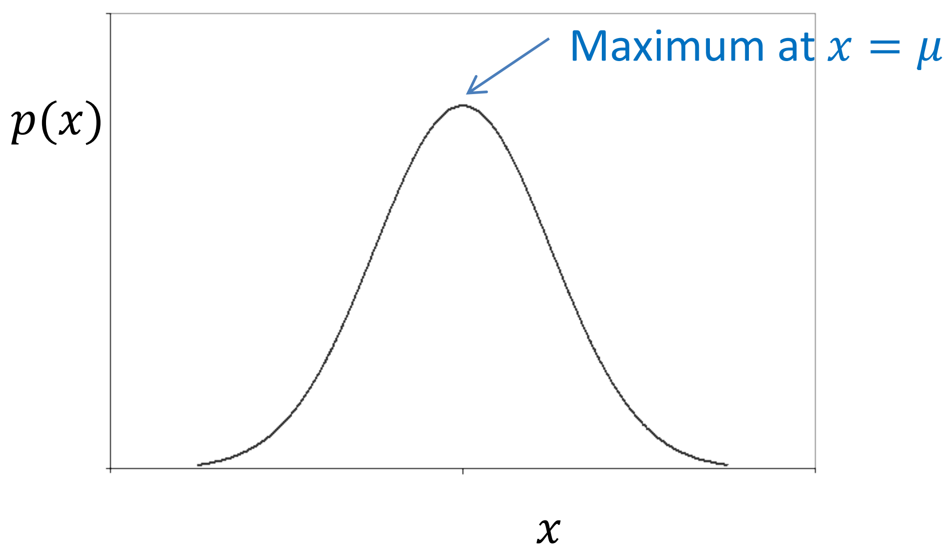
Typical prob distributions

- Gaussian distribution or normal distribution: over a continuous variable

$$\mathcal{N}(x;\mu,\sigma^2)=\sqrt{\frac{1}{2\pi\sigma^2}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

  - Mean: $\mathbb{E}[\mathrm{x}]=\mu$
  - Variance: $\mathrm{Var}[\mathrm{x}]=\sigma^2$
  - Standard deviation: σ

The *central limit theorem* shows that the sum of many independent variables is approximately normally distributed



Marginal probability

Suppose we know the prob distribution over a set of variables. The prob distribution over just a subset of them is known as the marginal prob distribution

- Let $P(\mathrm{x}, \mathrm{y})$ denote the prob distribution of discrete random variables x and y, then

$$P(\mathrm{x} = x) = \sum_{y} P(\mathrm{x} = x, \mathrm{y} = y)$$

- Let $p(\mathrm{x}, \mathrm{y})$ denote the PDF of continuous random variables x and y, then

$$p(x) = \int P(x, y) dy$$

Conditional probability

The conditional probability is the probability of some event, given that some other event has happened

- The conditional prob that $\mathrm{y} = y$ given $\mathrm{x} = x$ is denoted by $P(\mathrm{y} = y | \mathrm{x} = x)$, which can be calculated as
$$P(\mathrm{y} = y | \mathrm{x} = x) = P(\mathrm{y} = y, \mathrm{x} = x) / P(\mathrm{x} = x)$$
- The chain rule
$$P\left(\mathrm{x}^{(1)}, \dots, \mathrm{x}^{(n)}\right) = P\left(\mathrm{x}^{(n)}\right) \Pi_{i=1}^{n-1} P\left(\mathrm{x}^{(i)} \middle| \mathrm{x}^{(i+1)}, \dots, \mathrm{x}^{(n)}\right)$$
- Exercise: Is the following correct?
$$P(\mathrm{a}, \mathrm{b}, \mathrm{c}) = P(\mathrm{a} | \mathrm{b}, \mathrm{c}) P(\mathrm{b} | \mathrm{c}) P(\mathrm{c})$$

Expectation

The expectation, or expected value, of some function $f(x)$ w.r.t. a prob distribution $P(\mathrm{x})$ is the average value that f takes on when x is drawn from P

- For discrete variables

$$\mathbb{E}_{\mathrm{x}\sim P}[f(x)] = \sum_{x} P(x)f(x)$$

- For continuous variables

$$\mathbb{E}_{\mathrm{x}\sim P}[f(x)] = \int p(x)f(x)dx$$

- If the identity of the distribution is clear, we may write $\mathbb{E}_{\mathrm{x}}[f(x)]$
- Expectation is linear: if α and β do not depend on x, then

$$\mathbb{E}_{\mathrm{x}}[\alpha f(x) + \beta g(x)] = \alpha \mathbb{E}_{\mathrm{x}}[f(x)] + \beta \mathbb{E}_{\mathrm{x}}[g(x)]$$

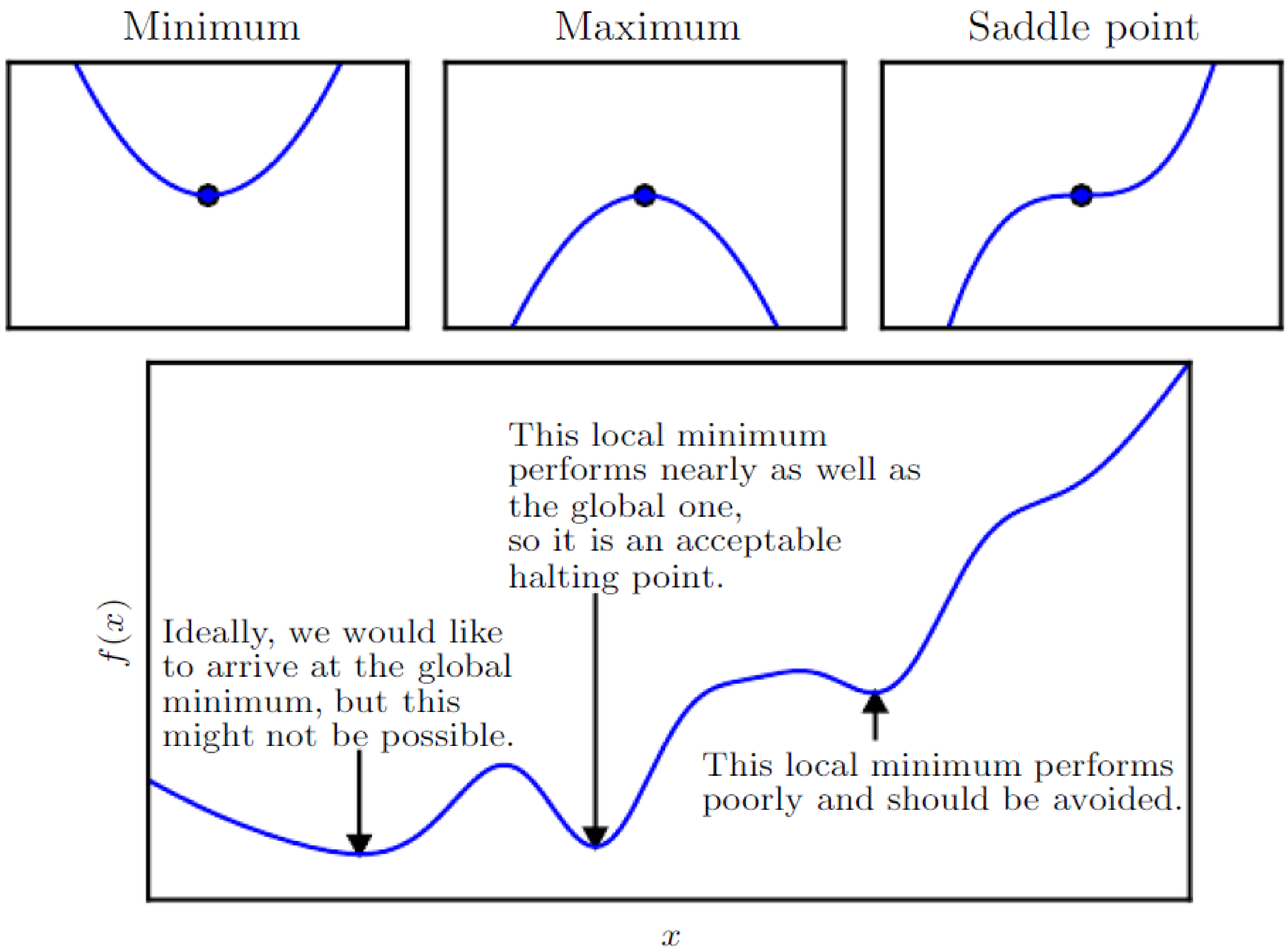
Gradient-based optimization

- The function we want to minimize or maximize is called objective function
- When we are minimizing it, we may also call it the cost function, loss function, or error function
- The derivative of a function $y = f(x)$, denoted by $f'(x)$ or $\frac{dy}{dx}$, gives the slope, or gradient, of f at the point x
- Gradient descent

$$x' = x - \eta f'(x)$$

where $\eta > 0$ is the learning rate

Critical points



Gradient decent for multivariate functions

- For a function of a single variable $y = f(x)$, the gradient decent method is
$$x' = x - \eta f'(x)$$
- For a function $y = f(\boldsymbol{x})$, the partial derivative is denoted by $\partial f / \partial x_i$
- The gradient decent method becomes
$$\boldsymbol{x}' = \boldsymbol{x} - \eta \nabla_{\boldsymbol{x}} f(\boldsymbol{x})$$

where $\eta > 0$ and $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \begin{pmatrix} \partial f / \partial x_1 \\ \partial f / \partial x_2 \\ \dots \\ \partial f / \partial x_n \end{pmatrix}$

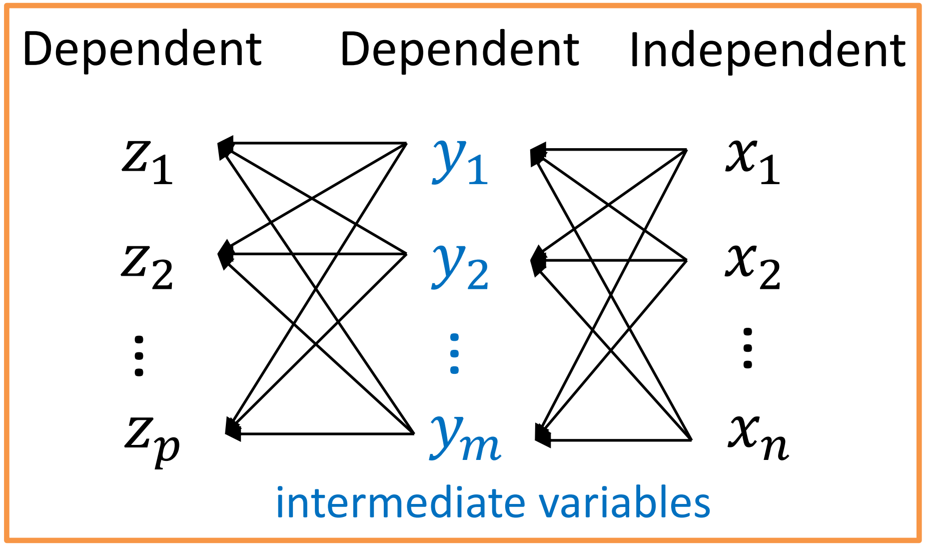
2D case

Rules in calculus

- Chain rule: the derivative of the composition function $f(g(x))$ is
$$[f(g(x))]' = f'(g(x))g'(x)$$
or in Leibniz's notation
$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$
- Product rule: the derivative of product of two functions
$$(f \cdot g)' = f' \cdot g + f \cdot g'$$
or in Leibniz's notation
$$\frac{d}{dx}(u \cdot v) = \frac{du}{dx} \cdot v + u \cdot \frac{dv}{dx}$$
- Quotient rule
$$\frac{d}{dx}\left(\frac{f(x)}{g(x)}\right) = \frac{f'g - fg'}{g^2}$$

Derivative of two-step composition

- Independent variables $x_1, x_2, \dots, x_n$
- Each y_i is a function of $x_1, x_2, \dots, x_n$
- Each z_i is a function of $y_1, y_2, \dots, y_m$



What's partial derivative of z_i w.r.t. x_j?

Derivative of two-step composition

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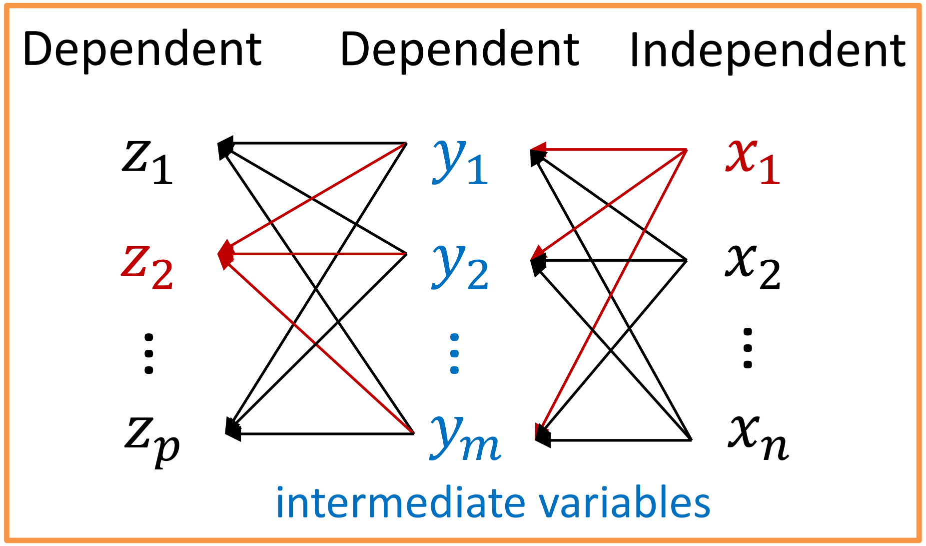

What's partial derivative of z_i w.r.t. x_j?

$$\frac{\partial z_2}{\partial x_1} = \frac{\partial z_2}{\partial y_1}\frac{\partial y_1}{\partial x_1} + \frac{\partial z_2}{\partial y_2}\frac{\partial y_2}{\partial x_1} + \cdots$$

$$\frac{\partial z_i}{\partial x_j} = \sum_{k=1}^{m} \frac{\partial z_i}{\partial y_k}\frac{\partial y_k}{\partial x_j}$$

Sum over the intermediate variables

for any $i \in \{1,2,\dots,p\}$ and $j \in \{1,2,\dots,n\}$

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Learning algorithms

"A computer program is said to learn from experience E w.r.t. some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E." ---Tom Mitchell, 1997

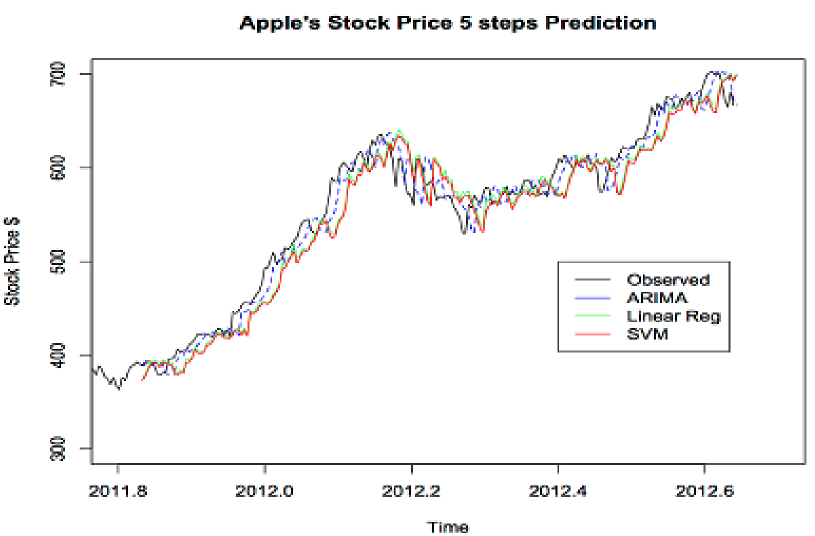
- Machine learning (ML) tasks are usually described in terms of how the ML system should process an example
- An example is a collection of features that have been quantitatively measured from some object or event
  - Features of a bucket: color, diameter, height, material, etc
  - Features of an animal: size, shape, number of legs, , etc






The tasks T

- Classification
  - Suppose there are k categories. Find a function $f: \mathbb{R}^n \rightarrow \{1, \dots, k\}$



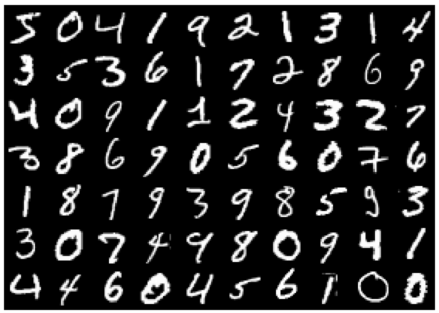
- Regression
  - Find a function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$, and m is often 1

Regression results might be converted to classification results

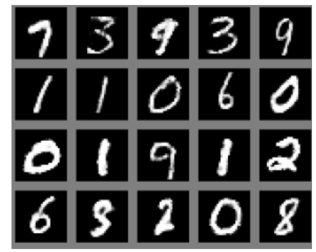
The tasks T

- Synthesis and sampling

dataset



Synthesized using GAN



- Denoising

The tasks T

- Transcription

Input

Output

Deep learning is cool

- Machine translation

The tasks, T

- Structured output
- Anomaly detection
- Synthesis and sampling
- Imputation of missing values
- Density estimation
- Etc.

The performance measure, P

- A performance measure is required to quantitatively evaluate the performance of a ML system
- Usually this measure P is specific to the task T being carried out by the system
  - Classification and transcription: accuracy or error rate
  - Regression and denoising: distance between the ground-truth and prediction
  - Synthesis, machine translation: difficult and sometimes need human evaluation
- What we are more interested in is the performance measure on a test set of data that is separated from the data used for training the system

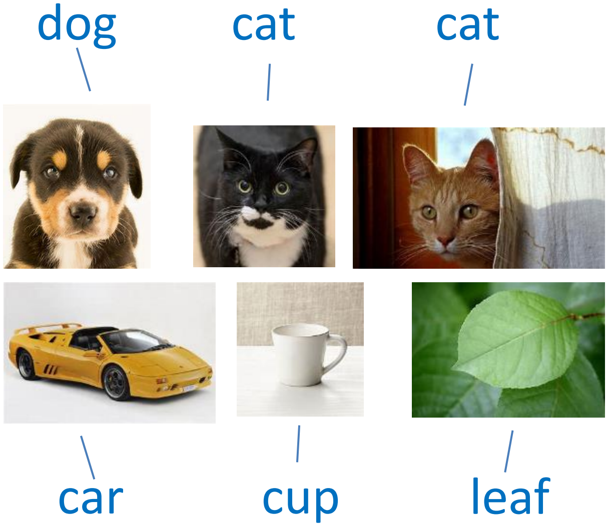
The experience, E

- ML algorithms can be broadly categorized as unsupervised and supervised by what kind of experience they are allowed to have during the learning process
- The algorithms experience a dataset, which is a collection of many examples or data points denoted by $\boldsymbol{x}$
  - We can view examples as samples of a random variable $\mathbf{x}$
- Unsupervised learning

learn $p(\mathbf{x})$

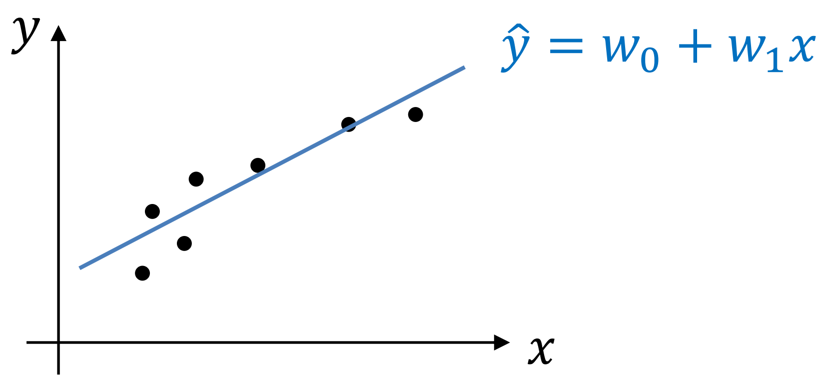
- Supervised learning algorithms

learn $p(\mathbf{y}|\mathbf{x})$



Example: linear regression

1D case



x_i: feature
w_i: weight

- Task T: to predict y from x by outputting $\hat{y} = \boldsymbol{w}^\top \boldsymbol{x}$
- Performance P: mean squared error of the model on the test with m test samples $\{(\boldsymbol{x}_i, y_i)\}^{\text{test}}$

$$\text{MSE}_{\text{test}} = \frac{1}{m} \sum_i (\hat{y}_i - y)^{\text{test}}$$

Example: linear regression

- Experience E: minimize the MSE on the training set of q samples $\{(\boldsymbol{x}_i, y_i)\}^{\text{train}}$

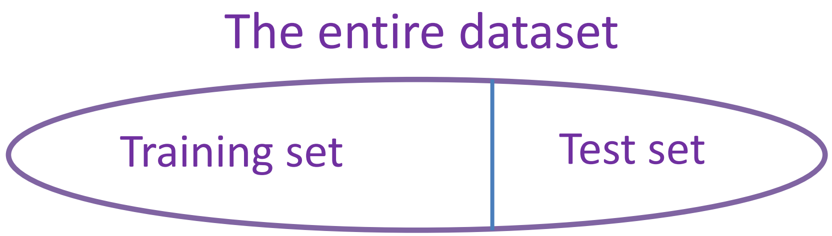
$$\text{MSE}_{\text{train}} = \frac{1}{q}\sum_i (\hat{y}_i - y)^{\text{train}}$$

  – Denote $\{(\boldsymbol{x}_i, y_i)\}^{\text{train}}$ collectively by $\left(\boldsymbol{X}^{\text{train}}, \boldsymbol{y}^{\text{train}}\right)$, then

$$\nabla_w \text{MSE}_{\text{train}} = \nabla_w \frac{1}{q}\left\|\hat{\boldsymbol{y}}^{\text{train}} - \boldsymbol{y}^{\text{train}}\right\|_2^2 = 0$$

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

Capacity, overfitting and underfitting



Large training error → low model capacity

Small training error → high model capacity

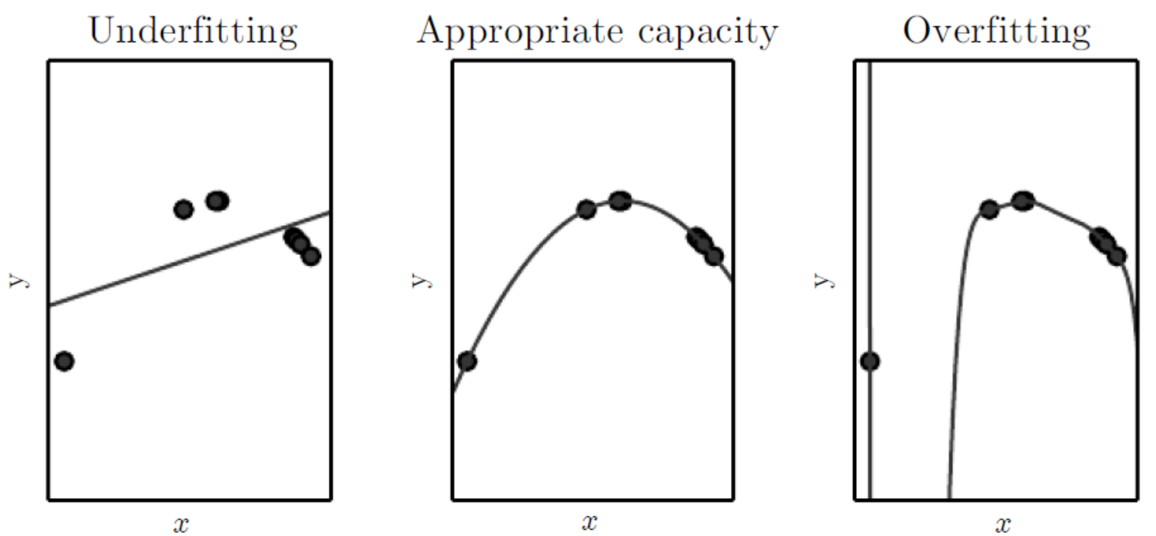
- What we want:
  - Small training error & small test error
  - If the training error is too large, the model is underfitting the training set
  - If the training error is very small but the test error is very large, the model is overfitting the training set
- A ML algorithm must perform well on new, previously unseen inputs
  - This ability is called generalization

Example: polynomial regression

- Consider a regression problem in which the input x and output y are both scalars. Find a function $f: \mathbb{R} \rightarrow \mathbb{R}$ to fit the data
  - $f(x) = b + wx$
  - $f(x) = b + w_1 x + w_2 x^2$
  - $f(x) = b + \sum_{i=1}^{9} w_i x^i$

MSE training:

$$\min_{w} \frac{1}{N} \sum_{n=1}^{N} \left\| f\left(x^{(n)}\right) - y^{(n)} \right\|_2^2$$



General principles

- Increase the model capacity
  - Make the training error small
- Increase the generalization ability
  - Make the gap between training error and test error small

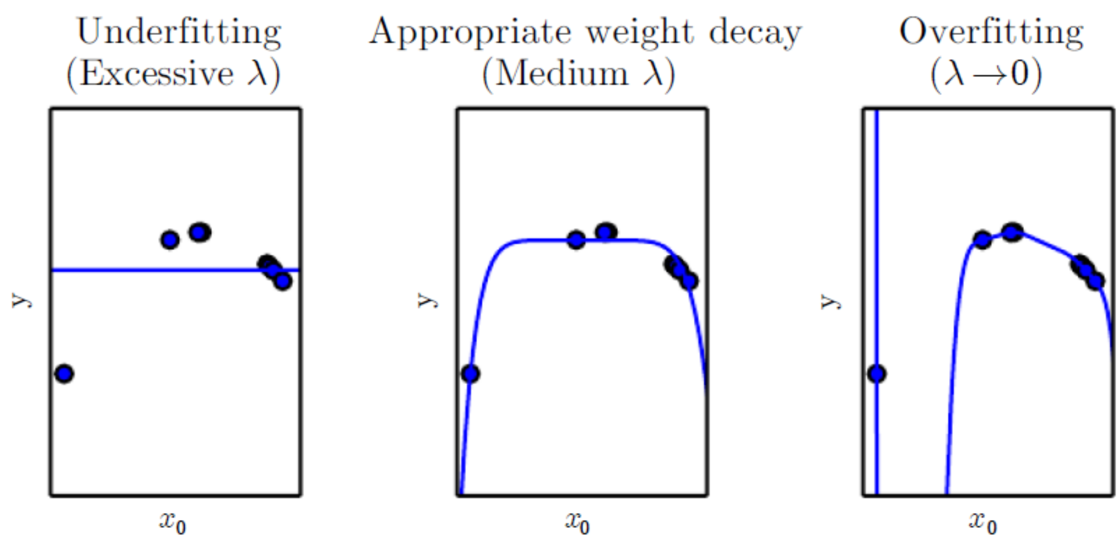
Regularization

- We often build a set of preferences into the learning algorithm, which is embodied by a regularizer Ω
- E.g., for polynomial regression, the total cost function becomes

$$J(\boldsymbol{w}) = \text{MSE}_{\text{train}} + \lambda \boldsymbol{w}^{\top}\boldsymbol{w}$$

Weight decay

where $\lambda > 0$ is a constant.



A high-degree polynomial regression example

- Here $\Omega(\boldsymbol{w}) = \boldsymbol{w}^{\top}\boldsymbol{w}$
- There are many regularizers

Regularization

Regularization is any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error

Hyperparameters

- Many machine learning algorithms have two sets of parameters:
  - Hyperparameters: control the algorithm's behavior and are not adapted by the algorithm itself. They often determines the capacity of the model
  - Learnable parameters ("learnable" is often omitted): can be learned from data
- The polynomial regression algorithm $J(\boldsymbol{w}) = \mathrm{MSE}_{\mathrm{train}} + \lambda \boldsymbol{w}^\top \boldsymbol{w}$
  - Hyperparameters: λ
  - Learnable parameters: $\boldsymbol{w}$

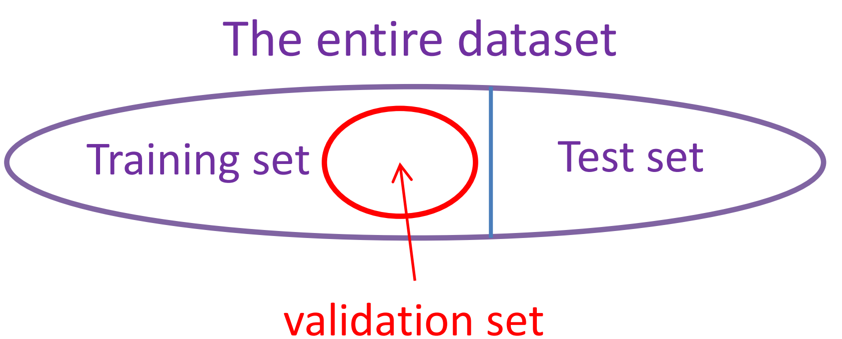
Question

- What are hyperparameters of a neural network?

- What are learnable parameters of a neural network?

Validation sets

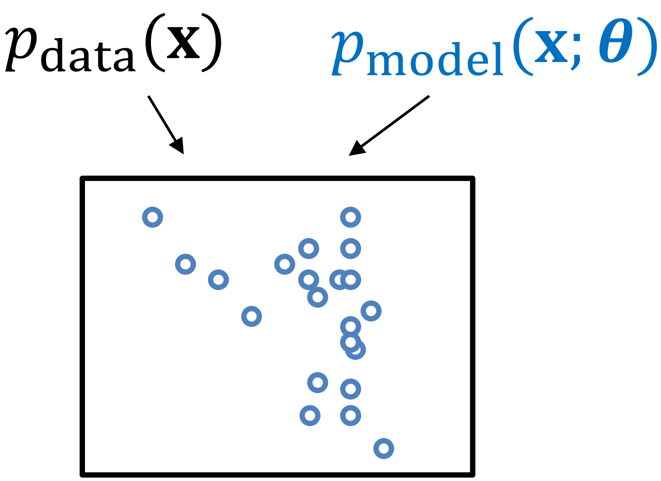
- How to choose the hyperparameters considering that we cannot see the test set?
  - Set them such that the training error is as small as possible?
- We need another set on which the model is not trained on
  - Make the error on this set as small as possible
  - This is called the validation set
- How do we obtain a validation set?



Maximum likelihood estimation (MLE)

Problem definition

- Given a set of N examples $\mathbb{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(N)}\}$ drawn independently from the true but unknown data-generating distribution $p_{\text{data}}(\mathbf{x})$
- Find a prob distribution $p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ to approximate $p_{\text{data}}(\mathbf{x})$
- Task: find optimal $\boldsymbol{\theta}$



Assumption:

The observed data samples $\mathbb{X}$ are generated from $p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ with the *maximum probability* over all possible $\boldsymbol{\theta}$

Maximum likelihood estimation (MLE)

Problem definition

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- Find a prob distribution $p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ to approximate $p_{\text{data}}(\mathbf{x})$
- Task: find optimal $\boldsymbol{\theta}$

- The MLE for $\boldsymbol{\theta}$ is defined as

$$\boldsymbol{\theta}_{\text{ML}} = \arg\max_{\boldsymbol{\theta}} p_{\text{model}}(\mathbb{X}; \boldsymbol{\theta}) = \arg\max_{\theta} \Pi_{i=1}^{N} p_{\text{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

- We usually use

$$\boldsymbol{\theta}_{\text{ML}} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{N} \log p_{\text{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

$$= \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{x}\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x}; \boldsymbol{\theta})$$

Log-likelihood

  - where $\hat{p}_{\text{data}}$ is the empirical distribution

Conditional log-likelihood

- Estimate a conditional probability $P(\mathbf{y}|\mathbf{x};\boldsymbol{\theta})$ in order to predict $\mathbf{y}$ given $\mathbf{x}$
  - E.g. For classification, $\mathbf{y}$ is a (discrete) random variable representing label of an input $\mathbf{x}$
- If $\boldsymbol{X}$ represents all inputs and $\boldsymbol{Y}$ all observed targets, then the conditional maximum likelihood estimator is

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\max_{\boldsymbol{\theta}} P_{\mathrm{model}}(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{\theta})$$

- If the examples are assumed to be i.i.d., then this can be decomposed into

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{N} \log P_{\mathrm{model}}(\boldsymbol{y}^{(i)}|\boldsymbol{x}^{(i)};\boldsymbol{\theta})$$

Stochastic gradient decent (SGD)

- Minimizing the cost function over the entire training set is computationally expensive
- Decompose the training set into minibatches and optimize the cost function $L(\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}; \boldsymbol{\theta})$ defined over individual minibatches $\left(\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}\right)$

> - $J(\boldsymbol{\theta}) = \sum_{i=1}^{N'} L(\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}; \boldsymbol{\theta})$
> - The batchsize ranges from 1 to a few hundreds

- At every iteration, update θ as follows

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \boldsymbol{g}'$$

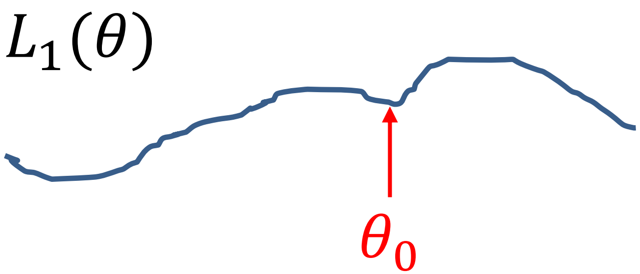
$$\boldsymbol{g}' = \nabla_{\boldsymbol{\theta}} L(\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}; \boldsymbol{\theta})$$

Advantages of SGD

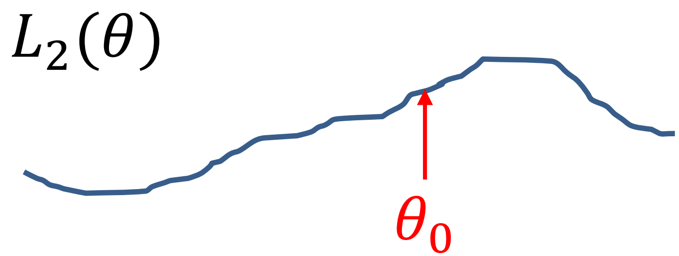
① Avoid large memory requirement when dealing with large training data

② Stochasticity is beneficial for escaping from "traps"

Note that $L(\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}; \boldsymbol{\theta})$ are different from different minibatches, so are their gradients



Local minimum



Not local minimum

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Summary of this lecture

I. Math basics

- PMF
- PDF
- Joint Prob
- Marginal prob
- Conditional prob
- Gradient decent

II. Machine learning basics

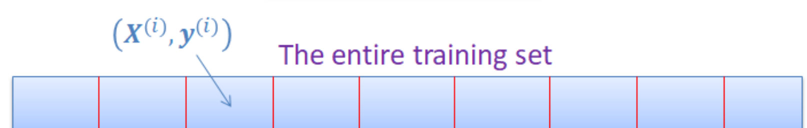
- Task T
- Performance P
- Experience E

Model capacity

MLE

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\max_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X}; \boldsymbol{\theta})$$

SGD



Recommended reading

- Chapters 2-5 in Deep Learning by Goodfellow, Bengio and Courville, 2016, MIT Press