Introduction to Deep Learning

Arijit Mondal
Dept. of Computer Science & Engineering
Indian Institute of Technology Patna
arijit@iitp.ac.in

Feature Engineering

Machine Learning

- A form of applied statistics with
  - Increased emphasis on the use of computers to statistically estimate complicated function
  - Decreased emphasis on proving confidence intervals around these functions
- Two primary approaches
  - Frequentist estimators
  - Bayesian inference

Types of Machine Learning Problems

- Supervised
- Unsupervised
- Other variants
  - Reinforcement learning
  - Semi-supervised

Learning algorithm

- A ML algorithm is an algorithm that is able to learn from data
- Mitchelle (1997)
  - A computer program is said to learn from experience E with respect to some class of task T and performance measure P, if its performance at task in T as measured by P, improves with experience E.

Task

- A ML tasks are usually described in terms of how ML system should process an example
  - Example is a collection of features that have been quantitatively measured from some objects or events that we want the learning system process
    - Represented as $\boldsymbol{x} \in \mathbb{R}^n$ where x_i is a feature
    - Feature of an image — pixel values

Common ML Task

- Classification
  - Need to predict which of the k categories some input belong to
  - Need to have a function $f : \mathbb{R}^n \rightarrow \{1, 2, \ldots, k\}$
  - $y = f(\boldsymbol{x})$ input $\boldsymbol{x}$ is assigned category identified by y
  - Examples
    - Object identification
    - Face recognition
- Regression
  - Need to predict numeric value for some given input
  - Need to have a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$
  - Examples
    - Energy consumption
    - Amount of insurance claim

Common ML Task (contd.)

- Classification with missing inputs
  - Need to have a set of functions
  - Each function corresponds to classifying $\boldsymbol{x}$ with different subset of inputs missing
  - Examples
    - Medical diagnosis (expensive or invasive)

Common ML Task (contd.)

- Classification with missing inputs
  - Need to have a set of functions
  - Each function corresponds to classifying $\boldsymbol{x}$ with different subset of inputs missing
  - Examples
    - Medical diagnosis (expensive or invasive)
- Transcription
  - Need to convert relatively unstructured data into discrete, textual form
    - Optical character recognition
    - Speech recognition

Common ML Task (contd.)

- Classification with missing inputs
  - Need to have a set of functions
  - Each function corresponds to classifying $\boldsymbol{x}$ with different subset of inputs missing
  - Examples
    - Medical diagnosis (expensive or invasive)
- Transcription
  - Need to convert relatively unstructured data into discrete, textual form
    - Optical character recognition
    - Speech recognition
- Machine translation
  - Conversion of sequence of symbols in one language to some other language
    - Natural language processing (English to Spanish conversion)

Common ML Task (contd.)

- Structured output
  - Output is a vector with important relationship between the different elements
    - Mapping natural language sentence into a tree that describes grammatical structure
    - Pixel based image segmentation (eg. identify roads)

Common ML Task (contd.)

- Structured output
  - Output is a vector with important relationship between the different elements
    - Mapping natural language sentence into a tree that describes grammatical structure
    - Pixel based image segmentation (eg. identify roads)
- Anamoly detection
  - Observes a set of events or objects and flags if some of them are unusual
    - Fraud detection in credit card

Common ML Task (contd.)

- Structured output
  - Output is a vector with important relationship between the different elements
    - Mapping natural language sentence into a tree that describes grammatical structure
    - Pixel based image segmentation (eg. identify roads)
- Anamoly detection
  - Observes a set of events or objects and flags if some of them are unusual
    - Fraud detection in credit card
- Synthesis and sampling
  - Generate new example similar to past examples
    - Useful for media application
    - Text to speech

Performance measure

- Accuracy is one of the key measures
  - The proportion of examples for which the model produces correct outputs
  - Similar to error rate
    - Error rate often referred as expected 0-1 loss
- Mostly interested how ML algorithm performs on unseen data
- Choice of performance measure may not be straight forward
  - Transcription
    - Accuracy of the system at transcribing entire sequence
    - Any partial credit for some elements of the sequence are correct

Experience

- Kind of experience allowed during learning process
  - Supervised
  - Unsupervised

Supervised learning

- Allowed to use labeled dataset
- Example — Iris
  - Collection of measurements of different parts of Iris plant
  - Each plant means each example
  - Features
    - Sepal length/width, petal length/width
    - Also record which species the plant belong to

Supervised learning (contd.)

- A set of labeled examples $\langle x_1, x_2, \ldots, x_n, y \rangle$
  - x_i are input variables
  - y output variable
- Need to find a function $f : X_1 \times X_2 \times \ldots X_n \rightarrow Y$
- Goal is to minimize error/loss function
  - Like to minimize over all dataset
  - We have limited dataset

Unsupervised learning

- Learns useful properties of the structure of data set
- Unlabeled data
  - Tries to learn entire probability distribution that generated the dataset
  - Examples
    - Clustering, dimensionality reduction

Supervised vs Unsupervised learning

- Unsupervised attempts to learn implicitly or explicitly probability distribution of $p(x)$
- Supervised tries to predict y from x ie. $p(y|x)$

Supervised vs Unsupervised learning

- Unsupervised attempts to learn implicitly or explicitly probability distribution of $p(x)$
- Supervised tries to predict y from x ie. $p(y|x)$
- Unsupervised learning can be decomposed as supervised learning

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, x_2, \ldots, x_{i-1})$$

Supervised vs Unsupervised learning

- Unsupervised attempts to learn implicitly or explicitly probability distribution of $p(\mathbf{x})$
- Supervised tries to predict $\mathbf{y}$ from $\mathbf{x}$ ie. $p(\mathbf{y}|\mathbf{x})$
- Unsupervised learning can be decomposed as supervised learning

$$p(\mathbf{x}) = \prod_{i=1}^{n} p(x_i | x_1, x_2, \ldots, x_{i-1})$$

- Solving supervised learning using traditional unsupervised learning

$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}, y)}{\sum_{y'} p(\mathbf{x}, y')}$$

Linear regression

- Prediction of the value of a continuous variable
  - Example — price of a house, solar power generation in photo-voltaic cell, etc.

Linear regression

- Prediction of the value of a continuous variable
  - Example — price of a house, solar power generation in photo-voltaic cell, etc.
- Takes a vector $\boldsymbol{x} \in \mathbb{R}^n$ and predict scalar $y \in \mathbb{R}$
  - Predicted value will be represented as $\hat{y} = \boldsymbol{w}^T\boldsymbol{x}$ where $\boldsymbol{w}$ is a vector of parameters
    - x_i receives positive weight — Increasing the value of the feature will increase the value of y
    - x_i receives negative weight — Increasing the value of the feature will decrease the value of y
    - Weight value is very high/large — Large effect on prediction

Performance

- Assume, we have m examples not used for training
  - This is known as test set

Performance

- Assume, we have m examples not used for training
  - This is known as test set
- Design matrix of inputs is $\boldsymbol{X}^{(\text{test})}$ and target output is a vector $\boldsymbol{y}^{(\text{test})}$
  - Performance is measured by Mean Square Error (MSE)

$$\text{MSE}_{(\text{test})} = \frac{1}{m}\sum_i \left(\hat{\boldsymbol{y}}^{(\text{test})} - \boldsymbol{y}^{(\text{test})}\right)_i^2 = \frac{1}{m}\|\hat{\boldsymbol{y}}^{(\text{test})} - \boldsymbol{y}^{(\text{test})}\|_2^2$$

  - Error increases when the Euclidean distance between target and prediction increases

Performance

- Assume, we have m examples not used for training
  - This is known as test set
- Design matrix of inputs is $\boldsymbol{X}^{(\text{test})}$ and target output is a vector $\boldsymbol{y}^{(\text{test})}$
  - Performance is measured by Mean Square Error (MSE)

$$\text{MSE}_{(\text{test})} = \frac{1}{m} \sum_i \left(\hat{\boldsymbol{y}}^{(\text{test})} - \boldsymbol{y}^{(\text{test})} \right)_i^2 = \frac{1}{m} \| \hat{\boldsymbol{y}}^{(\text{test})} - \boldsymbol{y}^{(\text{test})} \|_2^2$$

  - Error increases when the Euclidean distance between target and prediction increases
- The learning algorithm is allowed to gain experience from training set $(\boldsymbol{X}^{(\text{train})}, \boldsymbol{y}^{(\text{train})})$
- One of the common ideas is to minimize $\text{MSE}_{(\text{train})}$ for training set

Minimization of MSE

- We have the following now

$$\nabla_w \text{MSE}_{(\text{train})} = 0$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \mathrm{MSE}_{(\text{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \text{MSE}_{(\text{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \mathrm{MSE}_{(\mathrm{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\mathrm{train})} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})})^T (\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}) = 0
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \text{MSE}_{(\text{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})})^T (\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})}) = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})} \boldsymbol{w} - 2\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{y}^{(\text{train})} - \boldsymbol{y}^{(\text{train})T} \boldsymbol{y}^{(\text{train})}) = 0
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \mathrm{MSE}_{(\mathrm{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\mathrm{train})} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})})^T (\boldsymbol{X}^{(\mathrm{train})}\boldsymbol{w} - \boldsymbol{y}^{(\mathrm{train})}) = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{w}^T \boldsymbol{X}^{(\mathrm{train})T} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{w}^T \boldsymbol{X}^{(\mathrm{train})T} \boldsymbol{y}^{(\mathrm{train})} - \boldsymbol{y}^{(\mathrm{train})T} \boldsymbol{y}^{(\mathrm{train})}) = 0 \\
\Rightarrow \quad & 2\boldsymbol{X}^{(\mathrm{train})T} \boldsymbol{X}^{(\mathrm{train})} \boldsymbol{w} - 2\boldsymbol{X}^{(\mathrm{train})T} \boldsymbol{y}^{(\mathrm{train})} = 0
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \mathrm{MSE}_{(\text{train})} = 0 \\
\Rightarrow\ & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow\ & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow\ & \nabla_w (\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})})^T (\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - \boldsymbol{y}^{(\text{train})}) = 0 \\
\Rightarrow\ & \nabla_w (\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})}\boldsymbol{w} - 2\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{y}^{(\text{train})} - \boldsymbol{y}^{(\text{train})T} \boldsymbol{y}^{(\text{train})}) = 0 \\
\Rightarrow\ & 2\boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})}\boldsymbol{w} - 2\boldsymbol{X}^{(\text{train})T} \boldsymbol{y}^{(\text{train})} = 0 \\
\Rightarrow\ & \boldsymbol{w} = (\boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})})^{-1} \boldsymbol{X}^{(\text{train})} \boldsymbol{y}^{(\text{train})}
\end{aligned}
$$

Minimization of MSE

- We have the following now

$$
\begin{aligned}
& \nabla_w \mathrm{MSE}_{(\text{train})} = 0 \\
\Rightarrow \quad & \nabla_w \frac{1}{m} \|\hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \frac{1}{m} \nabla_w \|\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})}\|_2^2 = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})})^T (\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})}) = 0 \\
\Rightarrow \quad & \nabla_w (\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})} \boldsymbol{w} - 2\boldsymbol{w}^T \boldsymbol{X}^{(\text{train})T} \boldsymbol{y}^{(\text{train})} - \boldsymbol{y}^{(\text{train})T} \boldsymbol{y}^{(\text{train})}) = 0 \\
\Rightarrow \quad & 2\boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})} \boldsymbol{w} - 2\boldsymbol{X}^{(\text{train})T} \boldsymbol{y}^{(\text{train})} = 0 \\
\Rightarrow \quad & \boldsymbol{w} = (\boldsymbol{X}^{(\text{train})T} \boldsymbol{X}^{(\text{train})})^{-1} \boldsymbol{X}^{(\text{train})} \boldsymbol{y}^{(\text{train})}
\end{aligned}
$$

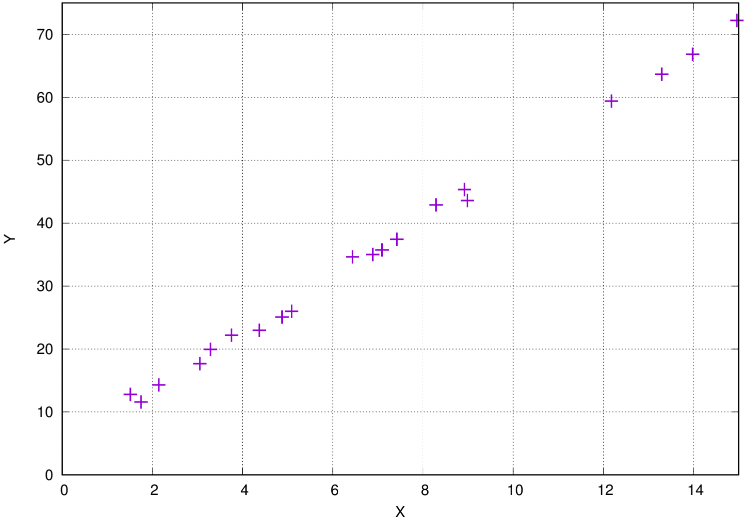
- Linear regression with bias term

$$\hat{y} = [\boldsymbol{w}^T \quad w_0][x \quad 1]^T$$

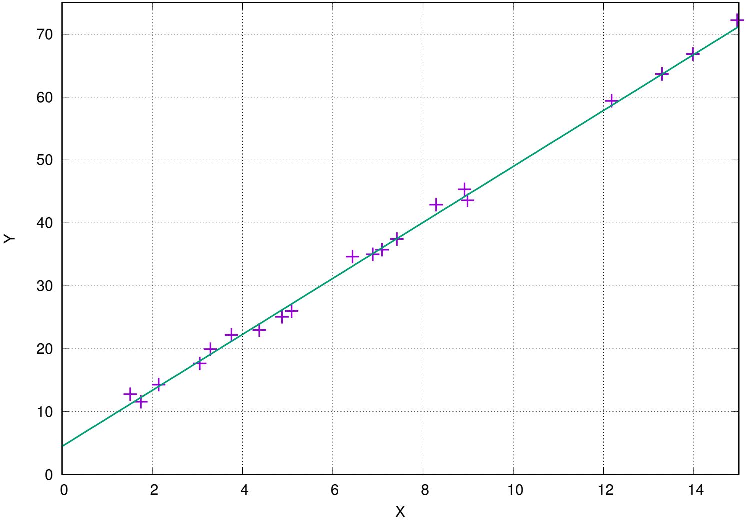
Moore-Penrose Pseudoinverse

- Let $\boldsymbol{A} \in \mathbb{R}^{n \times m}$
- Every $\boldsymbol{A}$ has pseudoinverse $\boldsymbol{A}^{+} \in \mathbb{R}^{m \times n}$ and it is unique
  - $\boldsymbol{A}\boldsymbol{A}^{+}\boldsymbol{A} = \boldsymbol{A}$
  - $\boldsymbol{A}^{+}\boldsymbol{A}\boldsymbol{A}^{+} = \boldsymbol{A}^{+}$
  - $(\boldsymbol{A}\boldsymbol{A}^{+})^{T} = \boldsymbol{A}\boldsymbol{A}^{+}$
  - $(\boldsymbol{A}^{+}\boldsymbol{A})^{T} = \boldsymbol{A}^{+}\boldsymbol{A}$
- $\boldsymbol{A}^{+} = (\boldsymbol{A}^{T}\boldsymbol{A})^{-1}\boldsymbol{A}^{T}$
- Example
  - If $\boldsymbol{A} = [1 \quad 2]^{T}$ then $\boldsymbol{A}^{+} = [\frac{1}{5} \quad \frac{2}{5}]$
  - If $\boldsymbol{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 5 \end{bmatrix}$ then $\boldsymbol{A}^{+} = \begin{bmatrix} 0.121212 & 0.515152 & -0.151515 \\ 0.030303 & -0.121212 & 0.212121 \end{bmatrix}$

Regression example



Regression example



Minimization of MSE: Gradient descent

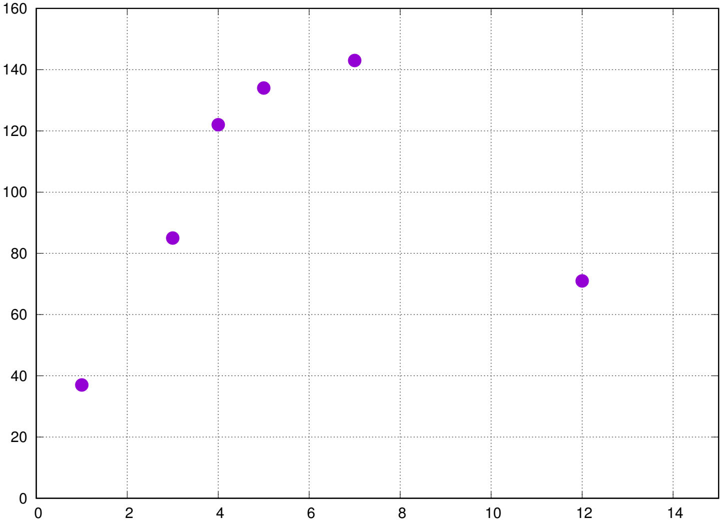
- Assuming $\text{MSE}_{(\text{train})} = J(w_1, w_2)$
- Target is to $\min\limits_{w_1, w_2} J(w_1, w_2)$
- Approach
  - Start with some w_1, w_2
  - Keep modifying w_1, w_2 so that $J(w_1, w_2)$ reduces till the desired accuracy is achieved

Minimization of MSE: Gradient descent

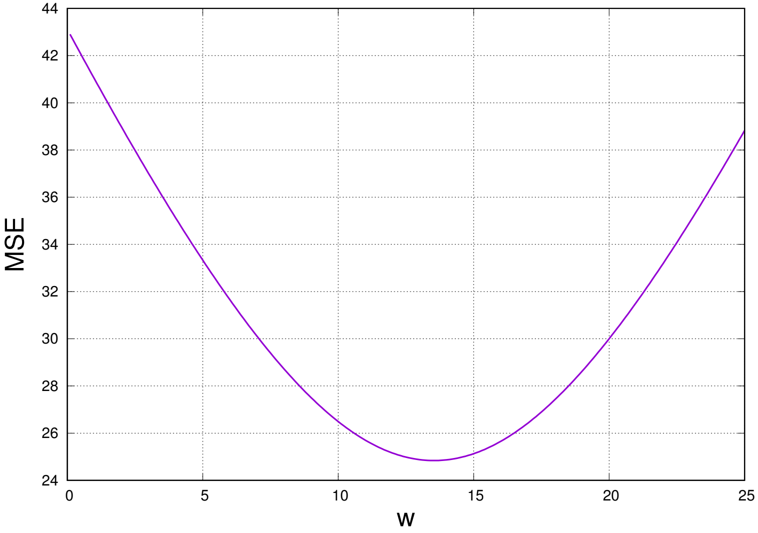
- Assuming $\text{MSE}_{(\text{train})} = J(w_1, w_2)$
- Target is to $\min\limits_{w_1, w_2} J(w_1, w_2)$
- Approach
    - Start with some w_1, w_2
    - Keep modifying w_1, w_2 so that $J(w_1, w_2)$ reduces till the desired accuracy is achieved
- Algorithm
    - Repeat the following until convergence

$$w_j = w_j - \frac{\partial}{\partial w_j} J(w_1, w_2)$$

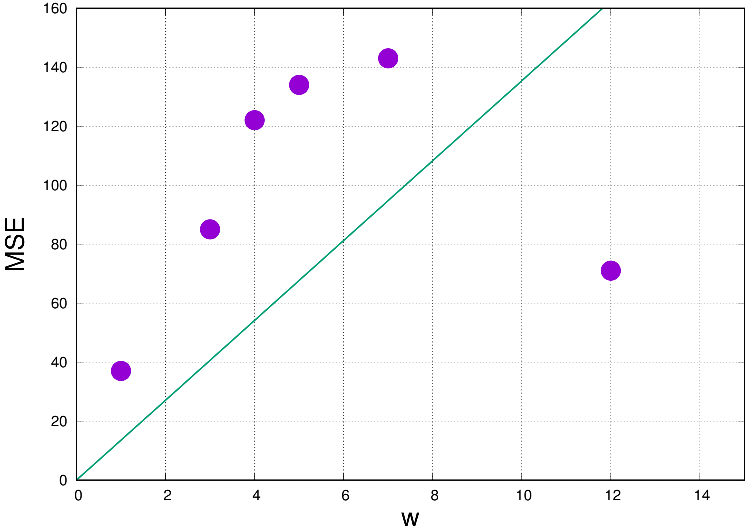
Example



Example



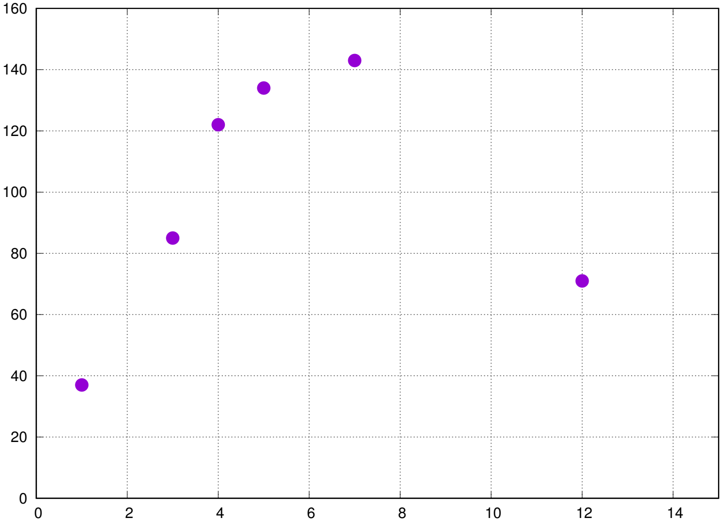
Example



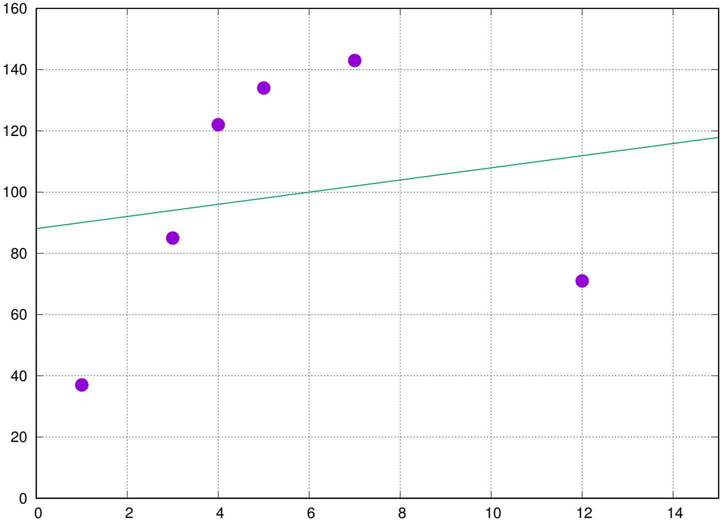
Error

- Training error - Error obtained on a training set
- Generalization error - Error on unseen data
- Data assumed to be independent and identically distributed (iid)
  - Each data set are independent of each other
  - Train and test data are identically distributed
- Expected training and test error will be the same
- It is more likely that the test error is greater than or equal to the expected value of training error
- Target is to make the training error is small. Also, to make the gap between training and test error smaller

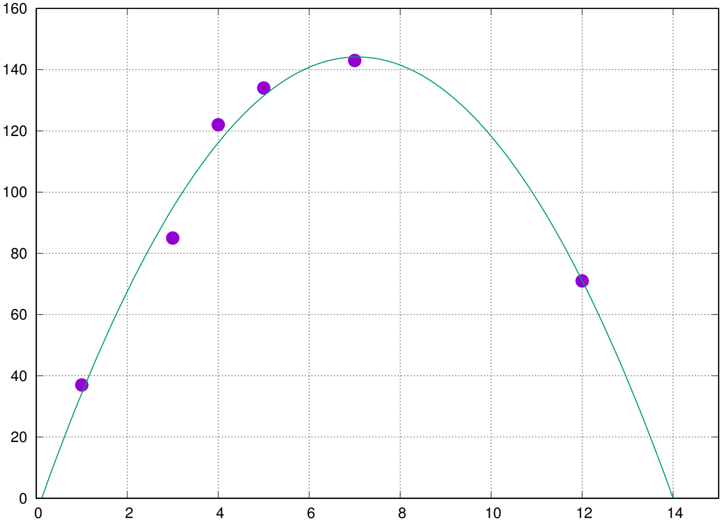
Regression example



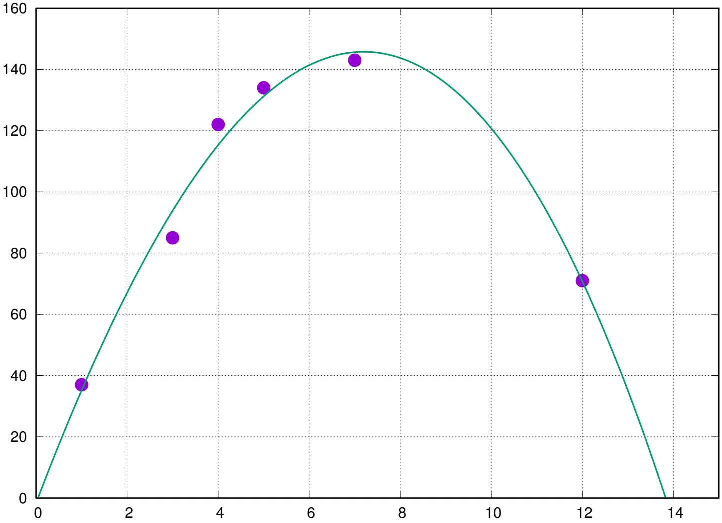
Regression example: degree 1



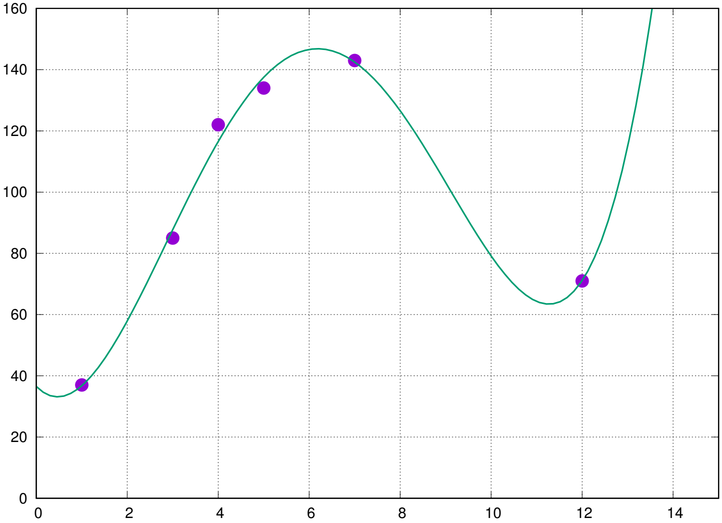
Regression example: degree 2



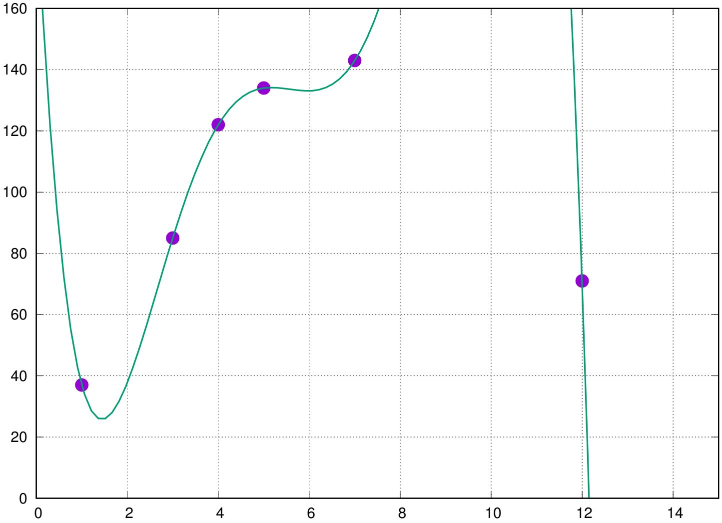
Regression example: degree 3



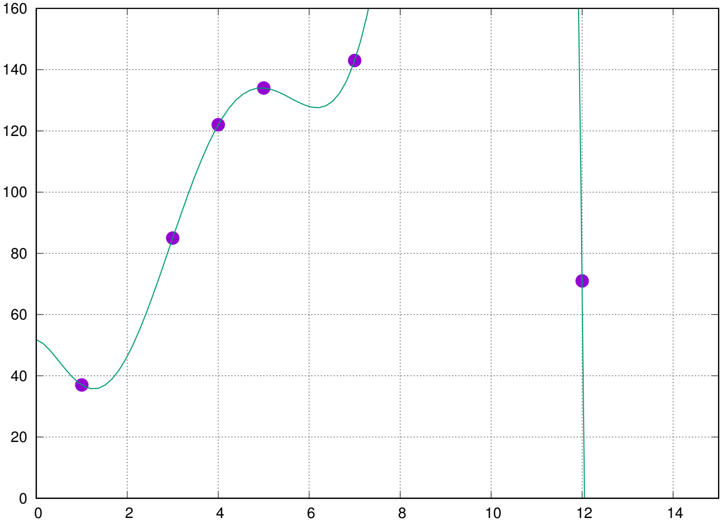
Regression example: degree 4



Regression example: degree 5



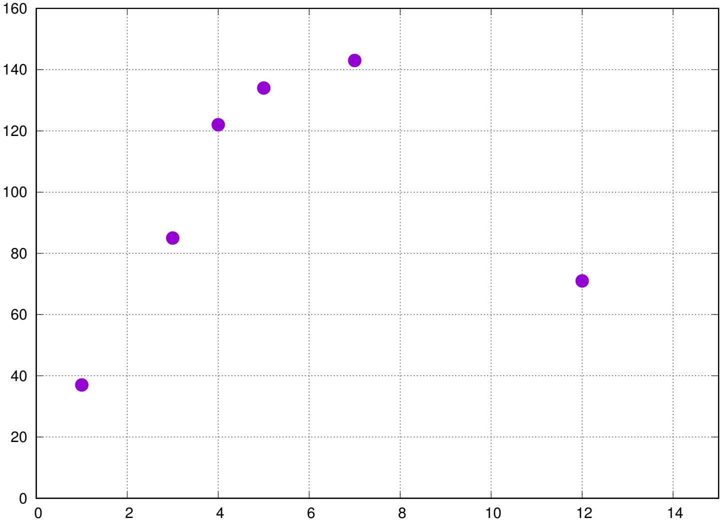
Regression example: degree 6



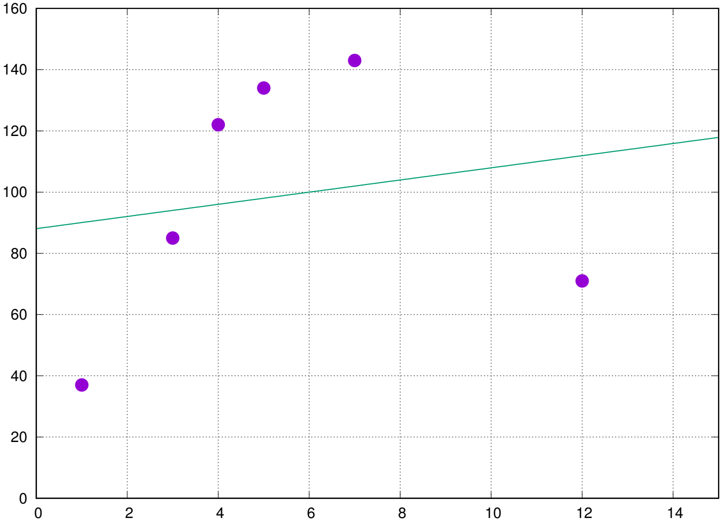
Underfitting & Overfitting

- Underfitting
  - When the model is not able to obtain sufficiently low error value on the training set
- Overfitting
  - When the gap between training set and test set error is too large

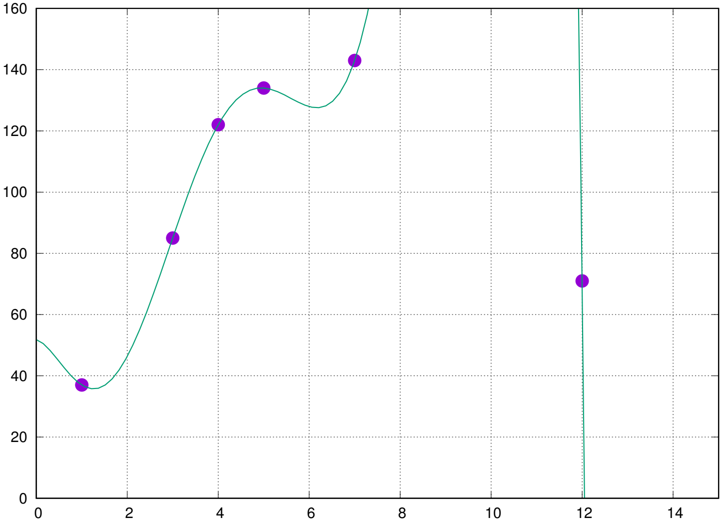
Example



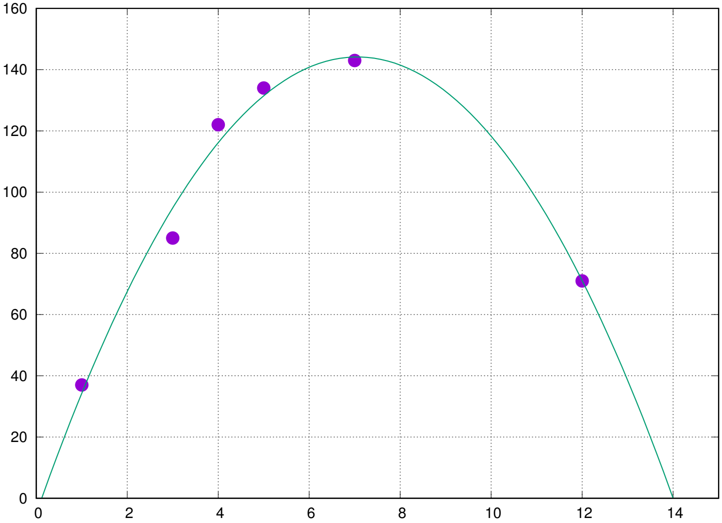
Underfitting example



Overfitting example



Better fit



Capacity

- Ability to fit wide variety of functions
  - Low capacity will struggle to fit the training set
  - High capacity will can overfit by memorizing the training set
- Capacity can be controlled by choosing hypothesis space
  - A polynomial of degree 1 gives linear regression $\hat{y} = b + wx$
  - By adding x^2 term, it can learn quadratic curve $\hat{y} = b + w_1 x + w_2 x^2$
    - Output is still a linear function of parameters
- Capacity of is determined by the choice of model (Representational capacity)
- Finding best function is very difficult optimization problem
  - Learning algorithm does not find the best function but reduces the training error
  - Imperfection in optimization algorithm can further reduce the capacity of model (effective capacity)

Capacity (contd.)

- Occam's razor
  - Among equally well hypotheses, choose the simplest one
- Vapnik-Chervonenski dimension - Capacity for binary classifier
  - Largest possible value of m for which a training set of m different $\boldsymbol{x}$ point that the classifier can label arbitrarily
- Training and test error is bounded from above by a quantity that grows as model capacity grows but shrinks as the number of training example increases
  - Bounds are usually provided for ML algorithm and rarely provided for DL
  - Capacity of deep learning model is difficult as the effective capacity is limited by optimization algorithm
    - Little knowledge on non-convex optimization

Error vs Capacity

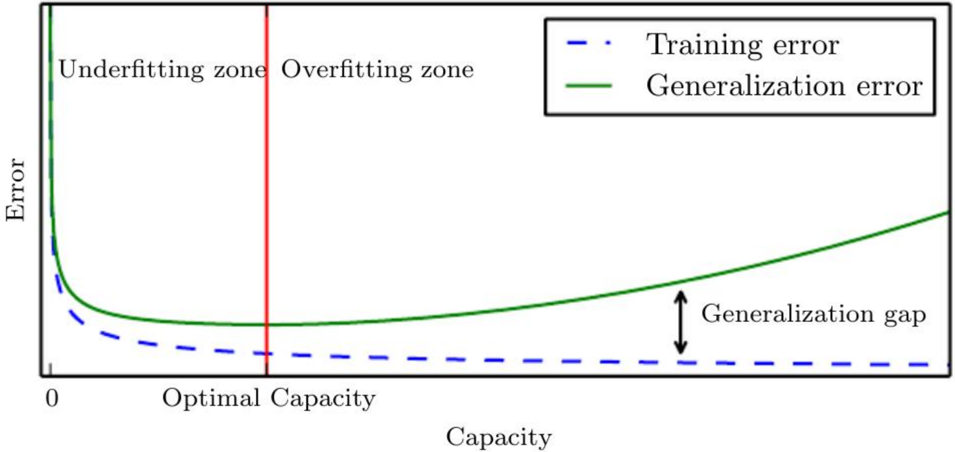


Image source: Deep Learning Book

Non-parametric model

- Parametric model learns a function described by a parameter vector
  - Size of vector is finite and fixed
- Nearest neighbour regression
  - Finds out the nearest entry in training set and returns the associated value as the predicted one
  - Mathematically, for a given point x, $\hat{y} = y_i$ where $i = \arg\min \|X_{i,:} - x\|_2^2$
- Wrapping parametric algorithm inside another algorithm

Bayes error

- Ideal model is an oracle that knows the true probability distribution for data generation
- Such model can make error because of noise
  - Supervised learning
    - Mapping of $\boldsymbol{x}$ to y may be stochastic
    - y may be deterministic but $\boldsymbol{x}$ does not have all variables
- Error by an oracle in predicting from the true distribution is known as Bayes error

Note

- Training and generalization error varies as the size of training set varies
- Expected generalization error can never increase as the number of training example increases
- Any fixed parametric model with less than the optimal capacity will asymptote to an error value that exceeds the Bayes error
- It is possible to have optimal capacity but have large gap between training and generalization error
  - Need more training examples

No free lunch

- Averaged over all possible data generating distribution, every classification algorithm has same error rate when classifying unseen points
- No machine learning algorithm is universally any better than any other

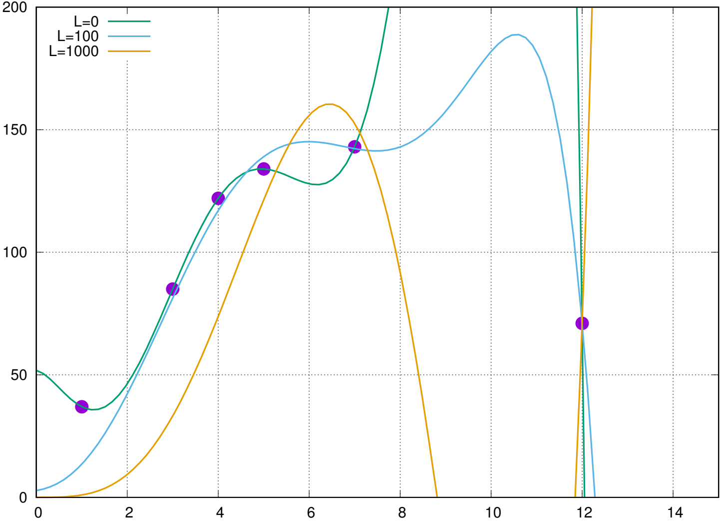
Regularization

- A set of preferences is applied to learning algorithm so that it perform well on a specific task
- Weight decay - In linear regression, preference on the weights is introduced
  - Sum of MSE and squared L^2 norms of the weight is minimized ie.

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

    - $\lambda = 0$ - No preference
    - λ becomes large - weight becomes smaller
- Regularization is intended to reduce test error not training error

Example: Weight decay



Hyperparameters

- Settings that are used to control the behavior of learning algorithm
  - Degree of polynomial
  - λ for decay weight
- Hyperparameters are usually not adapted or learned on the training set

Validation set

- Test data should not be used to choose the model as well as hyperparameters
- Validation set is constructed from training set
  - Typically 80% will be used for training and rest for validation
- Validation set may be used to train hyperparameters

Cross validation

- Dividing data set into training and fixed test may result into small test set
  - For large data this is not an issue
- For small data set use k-fold cross validation
  - Partition the data in k disjoint subsets
  - On i-th trial, i-th set used as the test set and rest are treated as training set
  - Test error can be determined by averaging the test error across the k trials

Point estimation

- To provide single best prediction of some quantity of interest
- Estimation of the relationship between input and output variables
- It can be single parameter or a vector of parameters
  - Weights in linear regression
- Notation: true parameter — $\boldsymbol{\theta}$ and estimate — $\hat{\boldsymbol{\theta}}$
- Let $\{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(m)}\}$ be set of m independent and identically distributed point.
- A point estimator is a function $\hat{\boldsymbol{\theta}}_m = g(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(m)})$
  - Good estimator is a function whose output is close to $\boldsymbol{\theta}$
  - $\boldsymbol{\theta}$ is unknown but fixed
  - $\hat{\boldsymbol{\theta}}$ depends on data

Bias

- Difference between this estimator's expected value and the true value of the parameter being estimated
  - $\text{bias}(\hat{\boldsymbol{\theta}}_m) = \mathbb{E}(\hat{\boldsymbol{\theta}}_m) - \boldsymbol{\theta}$
- An estimator will be said unbiased if $\text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$
  - $\mathbb{E}(\hat{\boldsymbol{\theta}}_m) = \boldsymbol{\theta}$
- An estimator will be asymptotically unbiased if $\lim_{m\to\infty} \text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \dfrac{1}{m} \sum_{i=1}^{m} x^{(i)}$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \dfrac{1}{m}\displaystyle\sum_{i=1}^{m} x^{(i)}$
- Bias of sample mean

$$\text{bias}(\hat{\mu}_m) \;=\; \mathbb{E}(\hat{\mu}_m) - \mu$$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$
- Bias of sample mean

$$\text{bias}(\hat{\mu}_m) \;=\; \mathbb{E}(\hat{\mu}_m) - \mu = \mathbb{E}\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right) - \mu$$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$
- Bias of sample mean

$$\text{bias}(\hat{\mu}_m) \;=\; \mathbb{E}(\hat{\mu}_m) - \mu = \mathbb{E}\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right) - \mu = \left(\frac{1}{m}\sum_{i=1}^{m} \mathbb{E}\left(x^{(i)}\right)\right) - \mu$$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \dfrac{1}{m}\sum_{i=1}^{m} x^{(i)}$
- Bias of sample mean

$$
\begin{aligned}
\text{bias}(\hat{\mu}_m) &= \mathbb{E}(\hat{\mu}_m) - \mu = \mathbb{E}\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right) - \mu = \left(\frac{1}{m}\sum_{i=1}^{m} \mathbb{E}\left(x^{(i)}\right)\right) - \mu \\
&= \left(\frac{1}{m}\sum_{i=1}^{m} \mu\right) - \mu
\end{aligned}
$$

Estimator for Gaussian distribution

- Let us consider a set of samples $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ that are independently and identically distributed according to $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$
- Gaussian mean estimator (also known as sample mean)
  - $\hat{\mu}_m = \dfrac{1}{m}\displaystyle\sum_{i=1}^{m} x^{(i)}$
- Bias of sample mean

$$
\begin{aligned}
\mathrm{bias}(\hat{\mu}_m) &= \mathbb{E}(\hat{\mu}_m) - \mu = \mathbb{E}\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right) - \mu = \left(\frac{1}{m}\sum_{i=1}^{m} \mathbb{E}\left(x^{(i)}\right)\right) - \mu \\
&= \left(\frac{1}{m}\sum_{i=1}^{m} \mu\right) - \mu = \mu - \mu = 0
\end{aligned}
$$

Estimator for Gaussian distribution (cont)

- Sample variance
  - $\hat{\sigma}_m^2 = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \hat{\mu}_m)^2$

Estimator for Gaussian distribution (cont)

- Sample variance
  - $\hat{\sigma}_m^2 = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \hat{\mu}_m)^2$
- Bias of sample variance $\text{bias}(\hat{\sigma}_m^2) = \mathbb{E}(\hat{\sigma}_m^2) - \sigma^2$
- It can be shown that, $\mathbb{E}(\hat{\sigma}_m^2) = \frac{m-1}{m}\sigma^2$

Trade off Bias and Variance

- Bias — Expected deviation from the true value of the function parameter
- Variance — Measure of deviation from the expected estimator value
- Choice of estimator — large bias or large variance?
  - Use cross-validation
  - Compare Mean Square Error

$$\mathrm{MSE} = \mathbb{E}(\hat{\theta}_m - \theta)^2 = \mathrm{bias}(\hat{\theta}_m)^2 + \mathrm{Var}(\hat{\theta}_m)$$

Trade off Bias and Variance (cont)

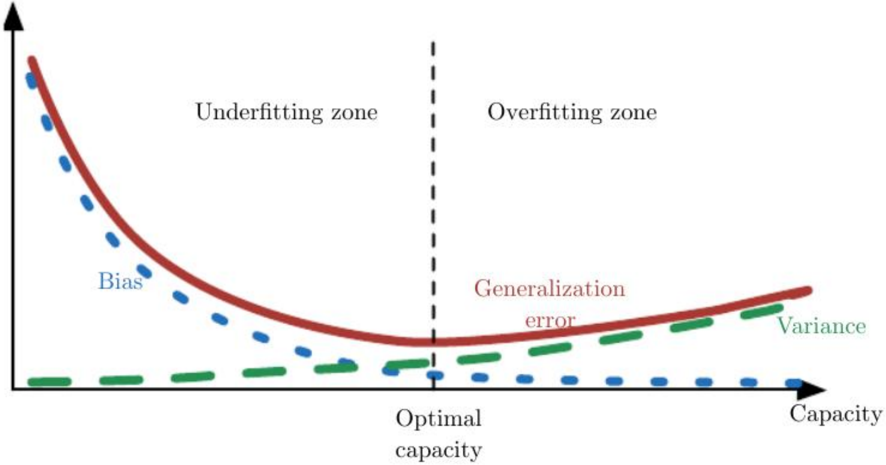


Image source: Deep Learning Book

Logistic regression

- Dependent variable is categorical
  - Example: $\langle$Hours of study, pass/fail$\rangle$
  - Output should lie between 0 and 1
  - Similar to linear regression except the output is mapped between 0 and 1 ie.

$$p(y|\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(x) = \dfrac{1}{1 + \exp(-x)}$ (Sigmoid function)

Support Vector Machine

- One of the most influential approaches for supervised learning
- A simple linear model $\boldsymbol{w}^T\boldsymbol{x} + b$ similar to logistic regression but does not provide probability
  - Predict positive class when $\boldsymbol{w}^T\boldsymbol{x} + b$ is positive and vice-versa
- Kernel trick

$$\boldsymbol{w}^T\boldsymbol{x} + b = b + \sum_{i=1}^{m} \alpha_i \boldsymbol{x}^T\boldsymbol{x}^{(i)} = b + \sum_{i=1}^{m} \alpha_i k(\boldsymbol{x}, \boldsymbol{x}^{(i)})$$

Challenges for Deep Learning

- Curse of dimensionality
- Local constancy and smoothness regularization
- Manifold learning