Introduction to Deep Learning

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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 task is 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 belongs to
  - Need to have a function $f : \mathbb{R}^n \rightarrow \{1, 2, \ldots, k\}$
  - $y = f(\boldsymbol{x})$ input $\boldsymbol{x}$ is assigned a 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 x with different subset of inputs missing
  - Examples
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    - Optical character recognition
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    - 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)

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- 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

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- **Supervised tries to predict** y **from** $\boldsymbol{x}$ **ie.** $p(y|\boldsymbol{x})$

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

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- Solving supervised learning using traditional unsupervised learning

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

Linear regression

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  - Example — price of a house, solar power generation in photo-voltaic cell, etc.

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- 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

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  - Performance is measured by Mean Square Error (MSE)

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

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

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

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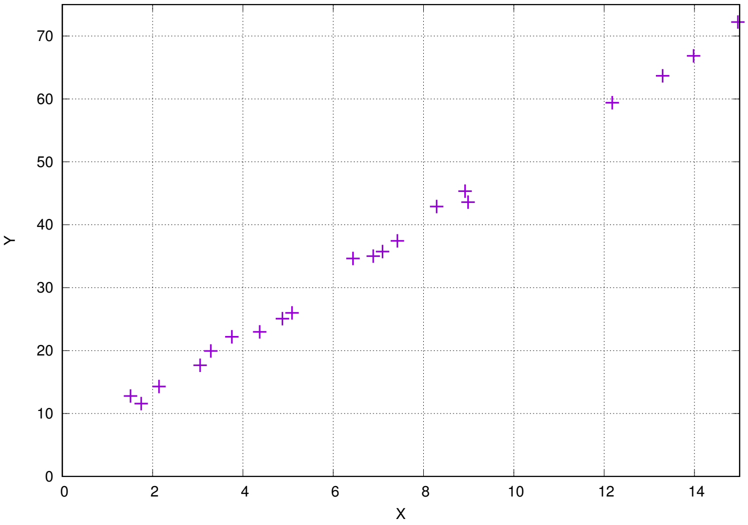
- Linear regression with bias term $\hat{y} = [\boldsymbol{w}^T \quad w_0][\boldsymbol{x} \quad 1]^T$

Moore-Penrose Pseudoinverse

- Let $A \in \mathbb{R}^{n \times m}$
- Every A has pseudoinverse $A^+ \in \mathbb{R}^{m \times n}$ and it is unique
  - $AA^+A = A$
  - $A^+AA^+ = A^+$
  - $(AA^+)^T = AA^+$
  - $(A^+A)^T = A^+A$
- $A^+ = \lim_{\alpha \to 0}(A^TA + \alpha I)^{-1}A^T$
- Example
  - If $A = [1 \quad 2]^T$ then $A^+ = [\frac{1}{5} \quad \frac{2}{5}]$
  - If $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 5 \end{bmatrix}$ then $A^+ = \begin{bmatrix} 0.121212 & 0.515152 & -0.151515 \\ 0.030303 & -0.121212 & 0.212121 \end{bmatrix}$

Regression example



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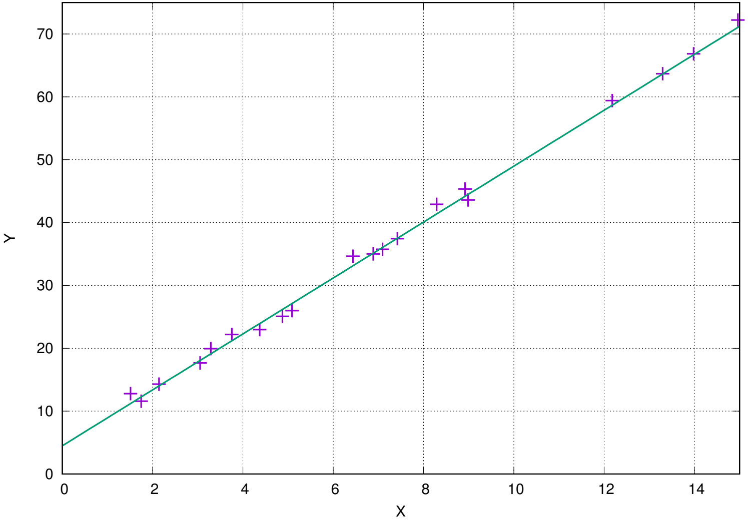

Minimization of MSE: Gradient descent

- Assuming $\text{MSE}_{(\text{train})} = J(w_1, w_2)$
- Target is to $\min_{w_1, w_2} J(w_1, w_2)$
- 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

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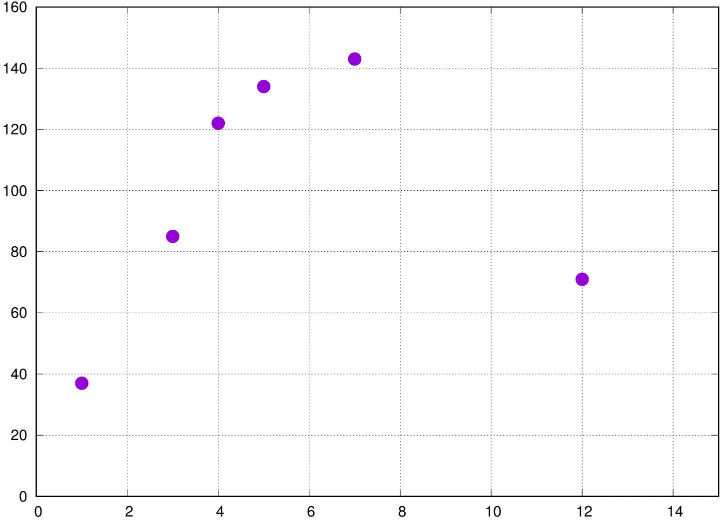
- Algorithm
  - Repeat the following until convergence

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

Example



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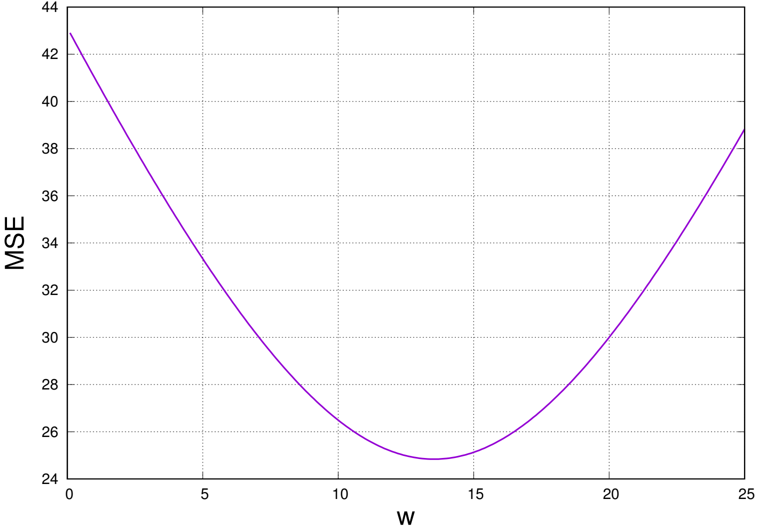

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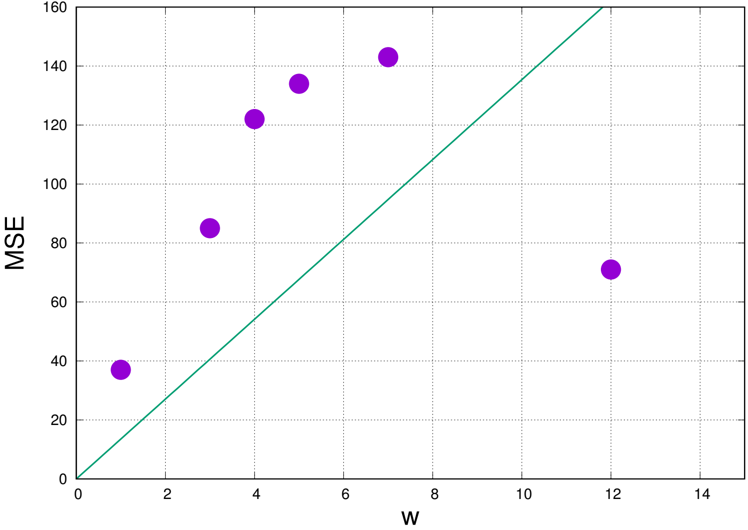
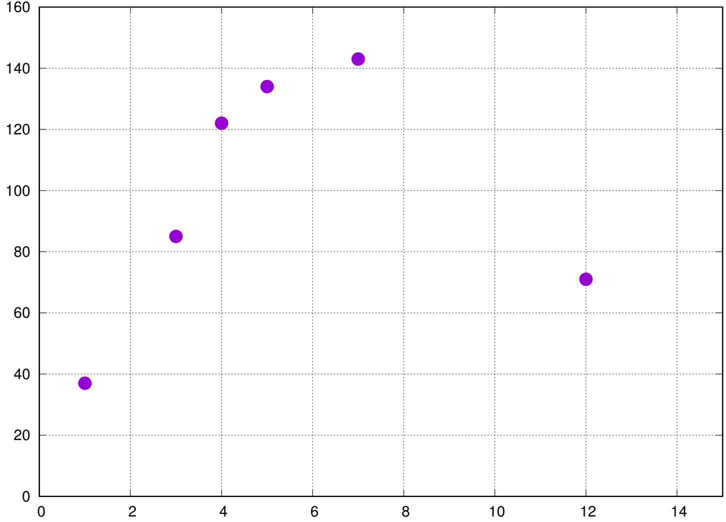


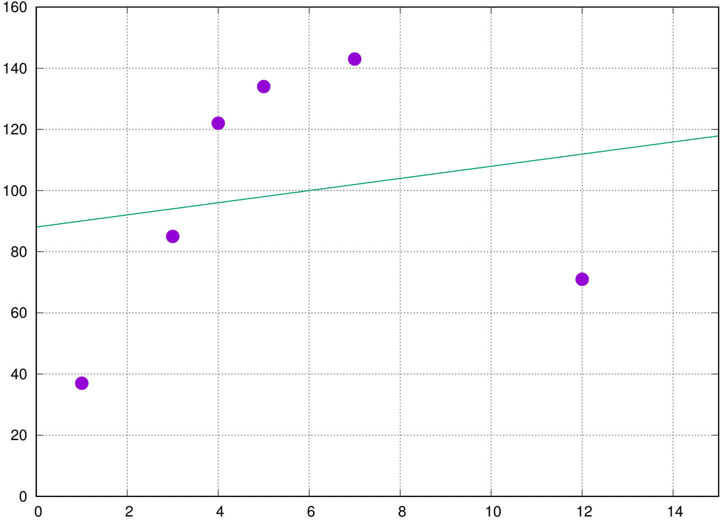
Error

- 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

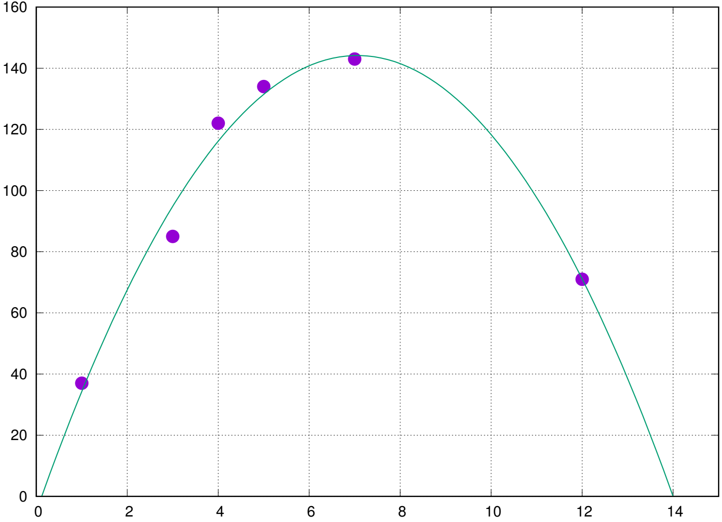
Regression example



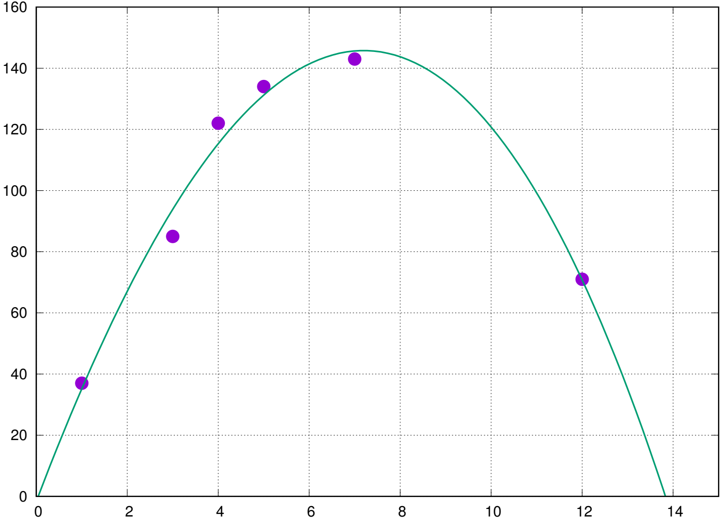
Regression example: degree 1



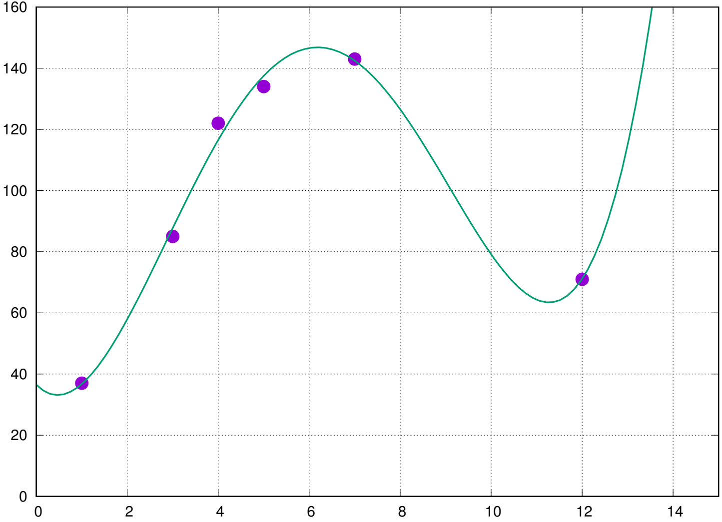
Regression example: degree 2



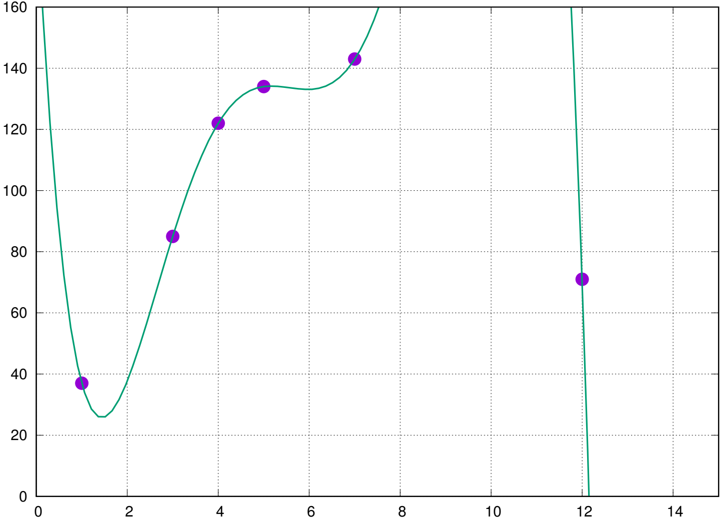
Regression example: degree 3



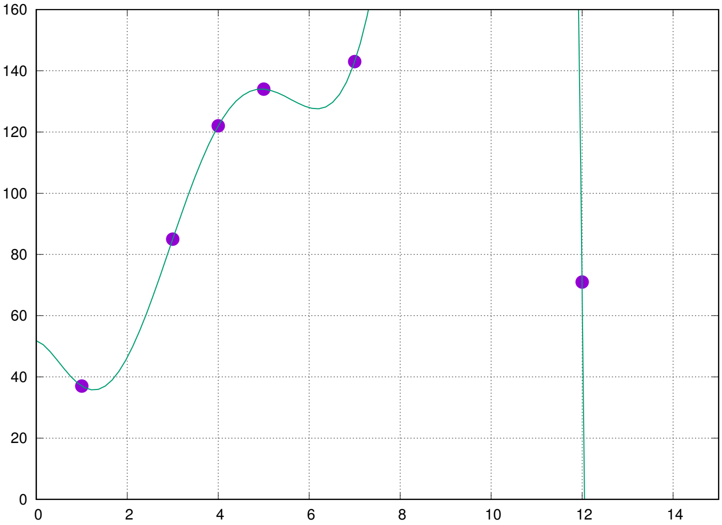
Regression example: degree 4



Regression example: degree 5



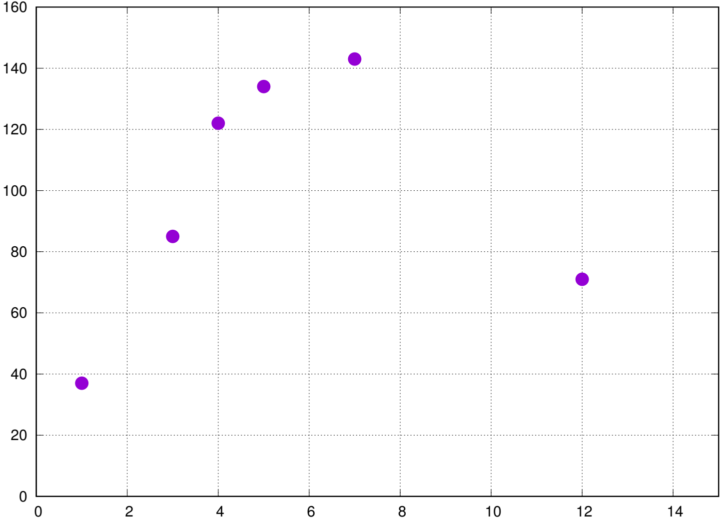
Regression example: degree 6



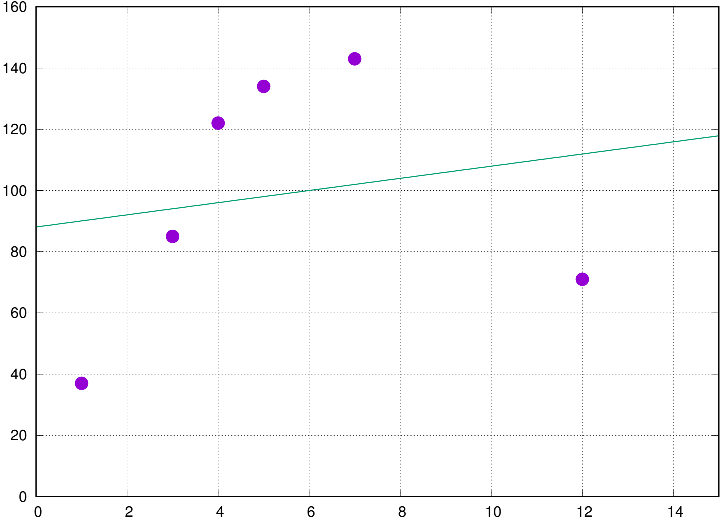
Underfitting & Overfitting

- 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

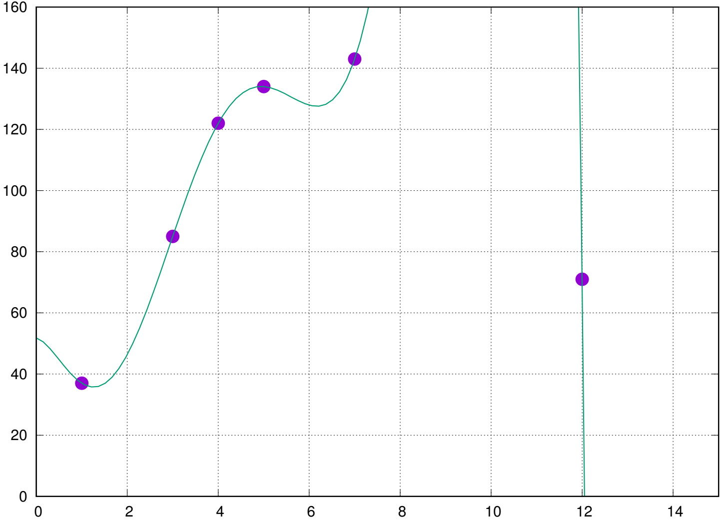
Example



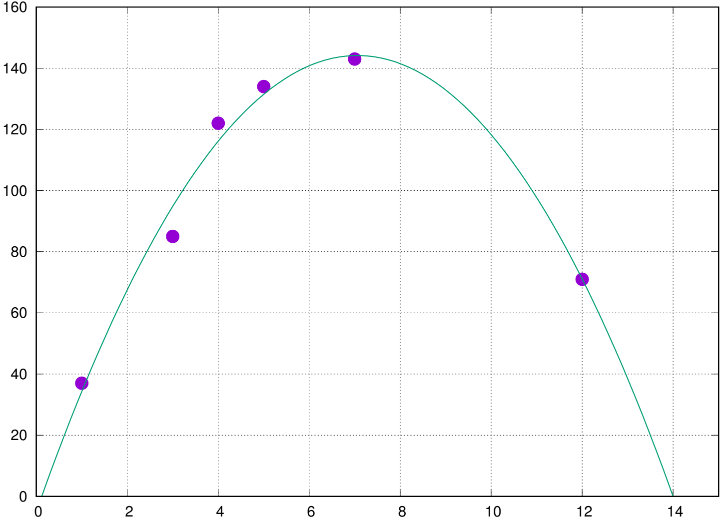
Underfitting example



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 $\hat{y} = b + w_1x + w_2x^2$
    - 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 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

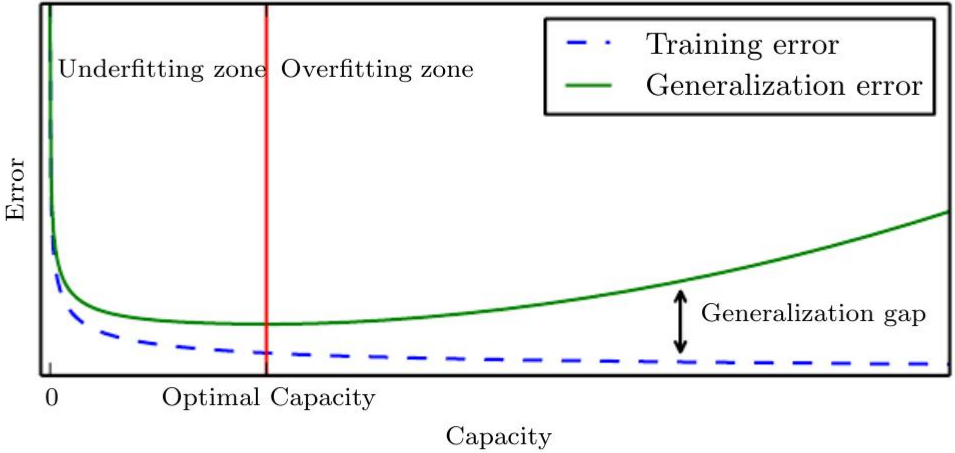


Image source: Deep Learning Book

Non-parametric model

- Parametric model learns a function described by a parameter vector
  - Size of vector is finite and fixed
- Nearest neighbor 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 x to y may be stochastic
    - y may be deterministic but 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

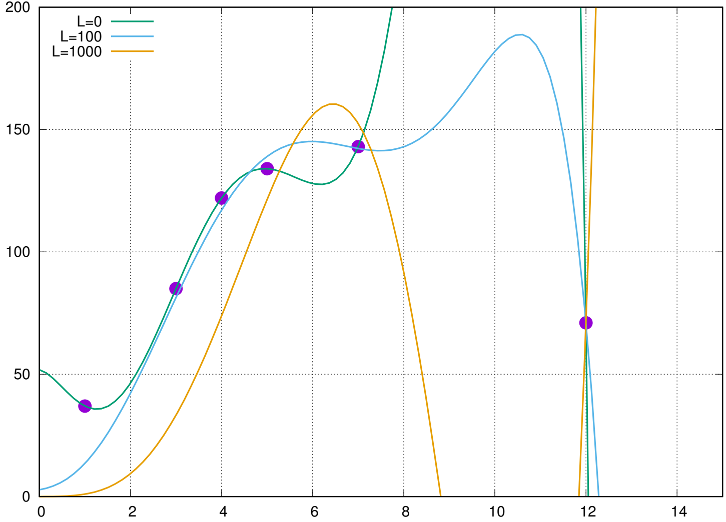
Regularization

- A set of preferences is applied to learning algorithm so that it performs 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.

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

    - $\lambda = 0$ - 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 — θ and estimate — $\hat{\theta}$
- 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 $\hat{\theta}_m = g(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(m)})$
  - Good estimator is a function whose output is close to θ
  - θ is unknown but fixed
  - $\hat{\theta}$ depends on data

Bias

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

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
  $p(x^{(i)}) = \mathcal{N}(x^{(i)}; \mu, \sigma^2) \quad \forall i = 1, 2, \ldots, m$

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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 $\textbf{bias}(\hat{\sigma}_m^2) = \mathbb{E}(\hat{\sigma}_m^2) - \sigma^2$
- 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**

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

Trade off Bias and Variance (cont)

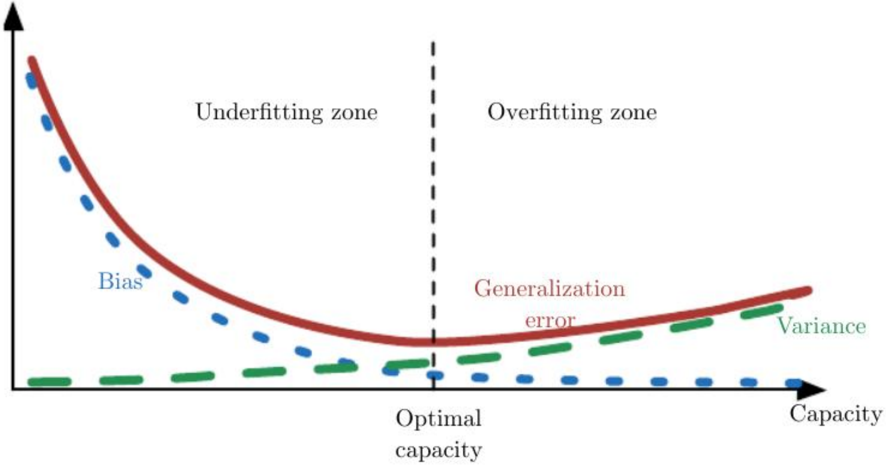
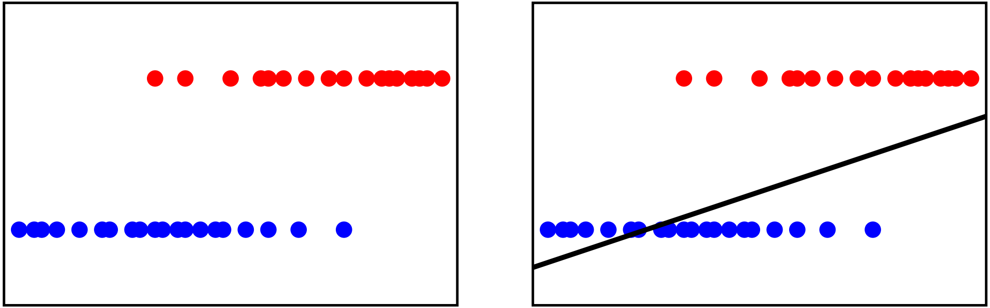


Image source: Deep Learning Book

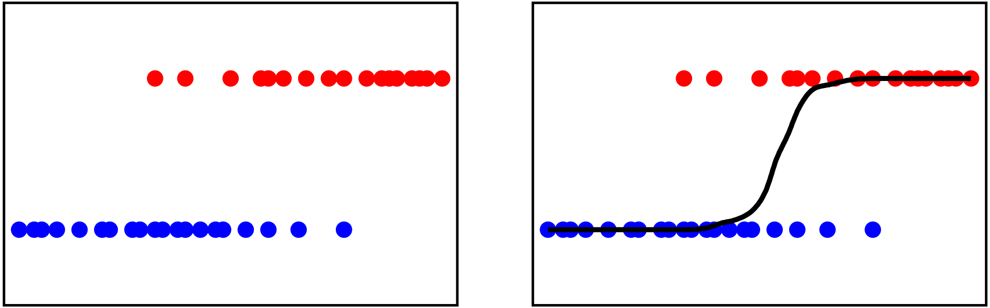
Logistic regression

- Responses may be qualitative (categorical)
  - Example: $\langle$Hours of study, pass/fail$\rangle$, $\langle$MRI scan, benign/malignant$\rangle$
  - Output should be 0 or 1
- Predicting qualitative response is known as classification
- Linear regression does not help

Issues with linear regression



Logistic regression



Logistic model

- **Linear regression model to represent probability** $p(x) = w_0 + w_1 x$
- **To avoid problem, we use function** $p(x) = \frac{e^{w_0 + w_1 x}}{1 + e^{w_0 + w_1 x}}$
- **Quantity** $\frac{p(x)}{1 - p(x)} = e^{w_0 + w_1 x}$ **is known as odds**
- **Taking** log **on both the sides, we get** $\log\left(\frac{p(x)}{1 - p(x)}\right) = w_0 + w_1 x$
- **Coefficient can be determined using maximum likelihood**
  - $l(w_0, w_1) = \prod_{i:y_i=1} p(x_i) \prod_{j:y_j=0} p(x_j)$

Logistic model (contd.)

- Similar to linear regression except the output is mapped between 0 and 1 ie.

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

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

Support Vector Machine

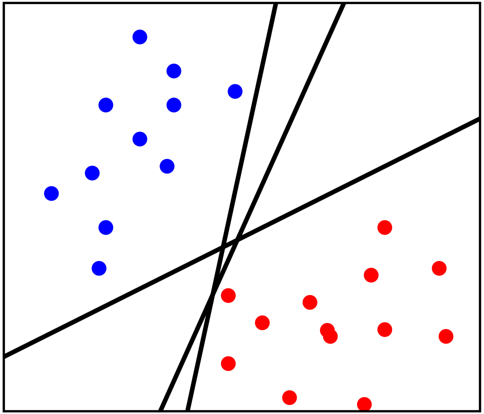
- An approach for classification
- Developed in 1990s
- Generalization of maximum margin classifier
  - Mostly limited to linear boundary
- Support vector classifier — broad range of classes
- SVM — Non-linear class boundary

Hyperplane

- In n dimensional space a hyperplane is a flat affine subspace of dimension $n-1$
- Mathematically it is defined as
  - For 2 dimensions — $w_0 + w_1x_1 + w_2x_2 = 0$
  - For n dimensions — $w_0 + w_1x_1 + \ldots + w_nx_n = 0$

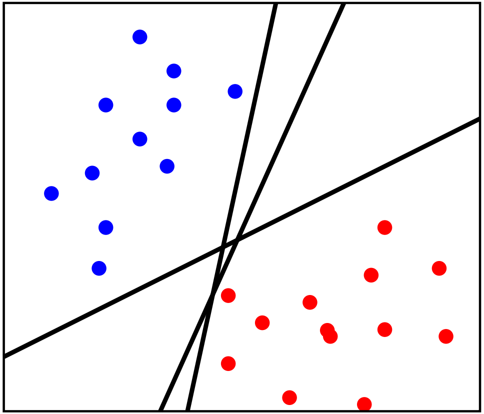
Classification using Hyperplane

- Assume, *m* training observation in *n* dimensional space



Classification using Hyperplane

- Assume, m training observation in n dimensional space
- Separating hyperplane has the property
  - $w_0 + w_1x_1 + \ldots + w_nx_n > 0$ **if** $y_i = 1$
  - $w_0 + w_1x_1 + \ldots + w_nx_n < 0$ **if** $y_i = -1$



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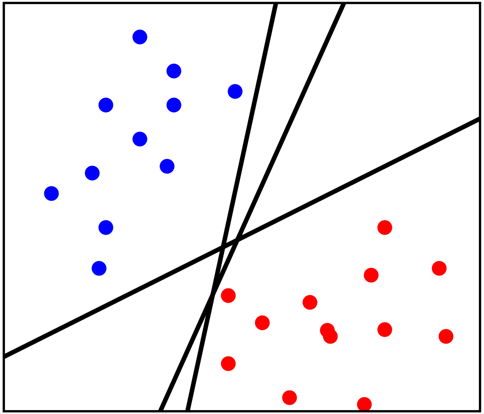
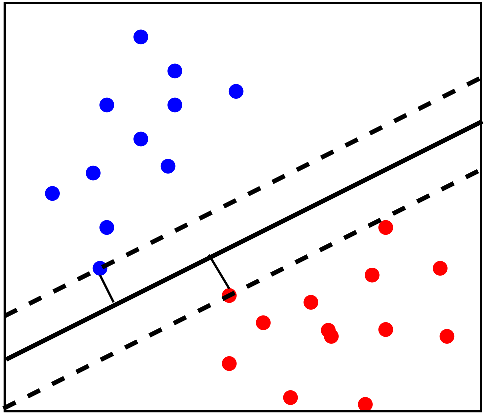
- Hence, $y_i(w_0 + w_1x_1 + \ldots + w_nx_n) > 0$
- Classification of test observation x^* is done based on the sign of

  $f(\boldsymbol{x}^*) = w_0 + w_1x_1^* + \ldots + w_nx_n^*$
- Magnitude of $f(\boldsymbol{x}^*)$
  - Far from 0 — Confident about prediction
  - Close to 0 — Less certain



Maximal margin classifier

- Also known as optimal separating hyperplane
- Separating hyperplane farthest from training observation
  - Compute perpendicular distance from training point to the hyperplane
  - Smallest of these distances represents the margin
- Target is to find the hyperplane for which the margin is the largest



Construction of maximal margin classifier

- Input — m points in n dimension space ie. $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m$
- Input — labels $y_1, y_2, \ldots, y_m$ for each point $\boldsymbol{x}_i$ where $y_i \in \{-1, 1\}$
- Need to solve the following optimization problem

$$\max_{w_0, w_1, \ldots, w_n, M} \quad M$$

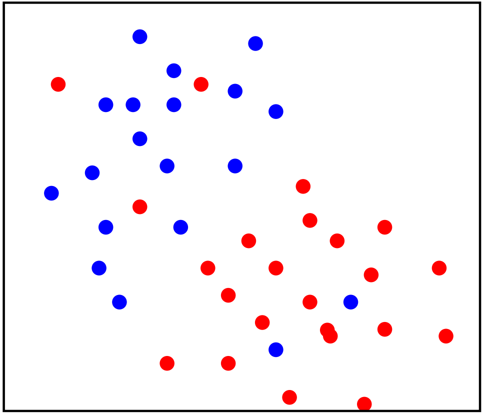
subject to

$$y_i(w_0 + w_1 x_{i1} + w_{i2} + \ldots + w_{in} x_{in}) \geq M \quad \forall i = 1, \ldots, m$$

$$\sum_{i=1}^{n} w_i^2 = 1$$

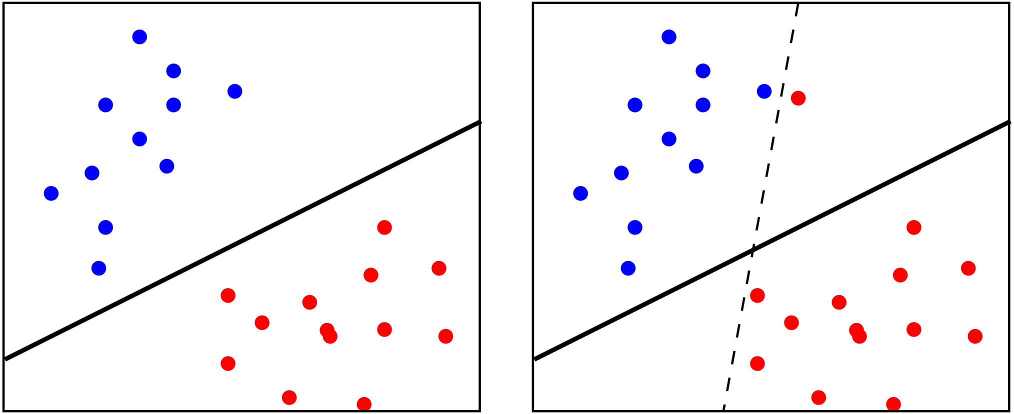
Issues

- Maximal margin classifier fails to provide classification in case of over-lap



Issues

- **Single observation point can change the hyperplane drastically**

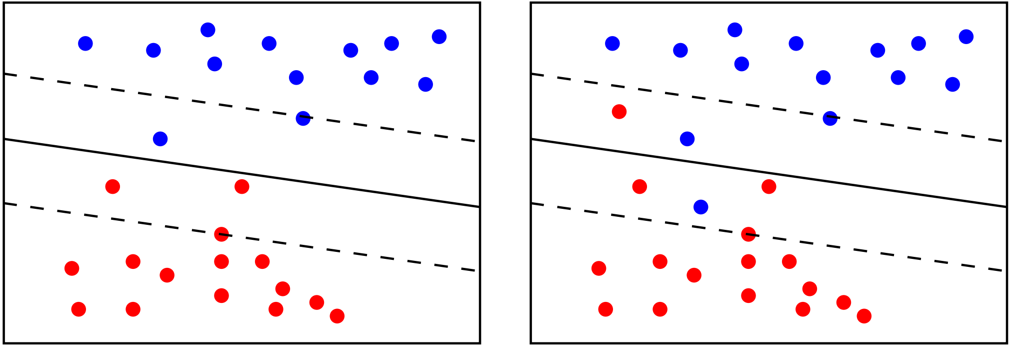


Support Vector Classifier

- Provides greater robustness to individual observations
- Better classification of most of the training observations
- Worthwhile to misclassify a few training observations
- Also known as soft margin classifier

Support Vector Classifier

- Points can lie within the margin or wrong side of hyperplane



Optimization with misclassification

- Input — $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$ and $y_1, y_2, \ldots, y_m$
- Need to solve the following optimization problem

$$\max_{w_0, w_1, \ldots, w_n, M} \quad M$$

subject to

$$y_i(w_0 + w_1 x_{i1} + \ldots + w_{in} x_{in}) \geq M(1 - \epsilon_i) \quad \forall i = 1, \ldots, m$$

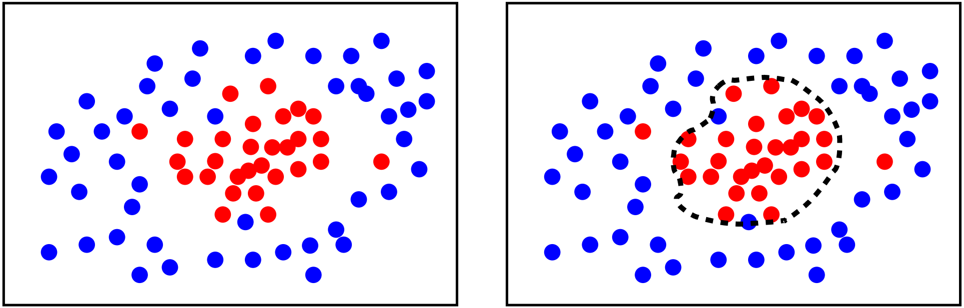
$$\sum_{i=1}^{n} w_i^2 = 1, \quad \sum_{i=1}^{m} \epsilon_i = C$$

- C is non-negative tuning parameter, ϵ_i - slack variable
- Classification of test observation remains the same

Observations

- $\epsilon_i = 0$ — ith observation is on the correct side of margin
- $\epsilon_i > 0$ — ith observation is on the wrong side of margin
- $\epsilon_i > 1$ — ith observation is on the wrong side of hyperplane
- C — budget for the amount that the margin can be violated by m observations
  - $C = 0$ — No violation, ie. maximal margin classifier
  - $C > 0$ — No more than C observation can be on the wrong side of hyperplane
  - C is small — Narrow margin, highly fit to data, low bias and high variance
  - C is large — Fitting data is less hard, more bias and may have less variance

Classification with non-linear boundaries



Classification with non-linear boundaries

- Performance of linear regression can suffer for non-linear data
- Feature space can be enlarged using function of predictors
  - For example, instead of fitting with $x_1, x_2, \ldots, x_n$ features we could use $x_1, x_1^2, x_2, x_2^2 \ldots, x_n, x_n^2$ as features
- Optimization problem becomes

$$\max_{w_0, w_{11}, w_{12} \ldots, w_{n1}, w_{n2}, \epsilon_i, M} \quad M$$

subject to

$$y_i \left(w_0 + \sum_{j=1}^{n} w_{j1} x_{ij} + \sum_{j=1}^{n} w_{j2} x_{ij}^2 \right) \geq M(1 - \epsilon_i) \quad \forall i = 1, \ldots, m$$

$$\sum_{i=1}^{n} \sum_{j=1}^{2} w_{ij}^2 = 1, \quad \sum_{i=1}^{m} \epsilon_i \leq C, \quad \epsilon_i \geq 0$$

Support Vector Machine

- **Extension of support vector classifier that results from enlarging feature space**

- **It involves inaner product of the observations** $f(x) = w_0 + \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle$

  where α_i **- one per training example**

  - **To estimate** α_i **and** w_0**, we need** $m(m-1)/2$ **inner products,** $\langle \mathbf{x}_i, \mathbf{x}_{i'} \rangle$

- **It turns out that** $\alpha_i \neq 0$ **for support vectors**

  $f(x) = w_0 + \sum_{i \in S} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle$ **where** S **- set of support vectors**

Support Vector Machine

- Inner product is replaced with kernel, K or $K(\mathbf{x}_i, \mathbf{x}_{i'})$
- Kernel quantifies similarity between observations $K(\mathbf{x}_i, \mathbf{x}_{i'}) = \sum_{j=1}^{n} x_{ij} x_{i'j}$
  - Above one is Linear kernel ie. Pearson correlation
- Polynomial kernel $K(\mathbf{x}_i, \mathbf{x}_{i'}) = \left(1 + \sum_{j=1}^{n} x_{ij} x_{i'j}\right)^d$ where d is positive integer > 1
- Support vector classifier with non-linear kernel is known as support vector machine and the function will look

$$f(x) = w_0 + \sum_{i \in S} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

- Radial kernel: $K(\mathbf{x}_i, \mathbf{x}_{i'}) = \exp\left(-\gamma \sum_{i=1}^{n} (x_{ij} - x_{i'j})^2\right)$ where $\gamma > 0$

Challenges for Deep Learning

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