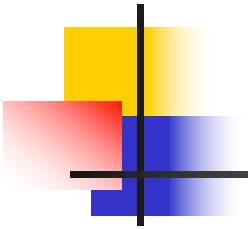


Machine Learning

Supervised Learning

Supervised Learning

- Supervised learning is learning where the training data contains the target output of the learning system.
  - Training data $D = \left\{ \left(x^{(i)}, y^{(i)} \right) : i \in \{1..n\} \right\}$
  - The type of output data determines the type of supervised learning problem
    - If *y* is a real number it is a regression problem
    - If *y* is an enumeration type it is a classification problem

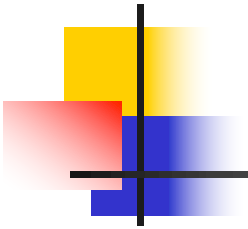
Supervised Learning

- The task of supervised learning is to learn a function (hypothesis), *h*, such that that $h(x^{(i)})$ is a "good" predictor for $y^{(i)}$: $h : X \rightarrow Y$
  - The representation used is an encoding of *h*
  - The hypothesis space is the space of all functions that can be represented with the representation
  - The evaluation/performance function determines what "good" means
  - When probabilistic criteria are used, *h* can also be chosen to represent *P(y)* followed by either a MLE,MAP, or expected value pick of y

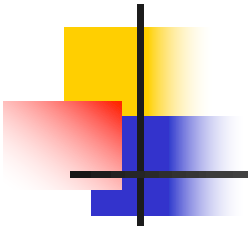
Supervised Learning Representations

- The space for all possible supervised learning solutions is the space of all functions
  - Infinitely large, requires infinite representation
    - It is intractable to design an algorithm with a universal and precise hypothesis space
      - Can limit the type of function
      - Can limit how precisely to represent the function
    - Parametric representations limit the type of function and encode the function using a set of parameters
    - Non-parametric functions limit the precision to which they model the function and represent it in terms of weighted data points

Supervised Learning Representations



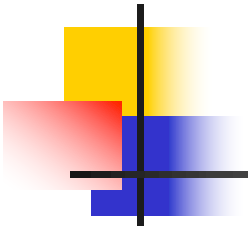
- Example representations include
  - Parametric
    - Polynomials of fixed degree
    - Parametric exponential functions
    - Neural networks
    - …
  - Non-parametric
    - Point-based density estimators
    - Point-based mixture distributions
    - Tile coding
    - …



Point-Based Estimators

- Point-based estimators are a non-parametric way to represent arbitrary functions with the precision limited by the number of points
  - Each data point represents the location of a specific (kernel) function and its weight represents the magnitude of its contribution
    - Kernel functions define the change in function value contribution when moving away from the point in terms of a similarity measure
  - The function estimate at another point is the sum or average of all the kernel functions' values at that point

Point-Based Probability Density Estimators



- To (approximately) represent an arbitrary probability density function we can use a point-based estimator where the kernel function is a valid probability density function and the weights are the probability of the point contributing (i.e. weights are a probability distribution over points)
  - At any point, the probability density is the weighted sum of the probability densities of the kernel functions at that point
    - The more points used, the more precise a function can be represented

Point-Based Probability Density Estimators

- Computation can be reduced by limiting how many points are used for any evaluation
  - If the kernel function has limited extent, we only need to use a subset of the points to estimate the density
    - E.g. Parzen window kernel

$$k(d/h) = \begin{cases} 1 & |d_i| \le 0.5 * h \\ 0 & otherwise \end{cases}$$

    - The expected number of points, n_V, contributing to any estimate is related to the probability density at that point and the size of the window, $V=h^D$

$$p(x) \approx \frac{n_V}{nV} = \frac{\sum_i k\left(\frac{x - x_i}{h}\right)}{n\, h^D}$$

Point-Based Probability Density Estimators

- Alternatively, the size of the kernel function can be regulated such that a constant number of points contribute to the estimate
  - Easiest using a hyperspherical window rather than a Parzen window

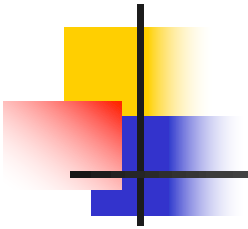
$$k(d/h) = \begin{cases} \dfrac{1}{V_h} & |d| \le h \\ 0 & otherwise \end{cases}$$

  - The value for h (and thus V) at a point is set such that exactly k data points fall within it. Then:

$$p(x) \approx \frac{k}{nV_{h(k)}}$$

Non-Parametric Supervised Learning – An Example

- One of the simplest machine learning approaches is K-Nearest Neighbor (KNN)
  - Given a set of (class) labeled data points and a query x $\{(x_1,c_1),\ldots, (x_n,c_n)\}$
    - Can also be used for regression problems
  - Pick the k data points most similar to x
  - Return the label that is associated with the largest number of the data points
- KNN is a supervised learning algorithm using a point-based density representation



KNN Classification

- What is the answer to the KNN learning problem ?
  - Data: {((1, 1); S),((2, 1); F),((2, 2); F),((1, 3); S),(3, 3; S)}; K=3; Point=(1.25, 1.75)
  - Answer:
    - Three nearest points (using Cartesian distance) are: ((1, 1); S), ((2, 2); F), ((2, 1); F)
    - Answer is F
  - Why is that a good answer ?
    - What would the elements of a formal learning algorithm be that gives us this solution ?

KNN Classification

- Representation
  - Hypothesis space:
    - Set of point-based class probability distributions
  - Representation:
    - sets of labeled data points and a distance/similarity measure forming a kernel-based probability distribution
      - In the simplest form the kernels are spherical windows
    - Data points represent limited range probability estimates supporting the class label

$$p(x \mid C) \approx \frac{k_C}{n_C V_{h(k)}}; p(x) \approx \frac{k}{n V_{h(k)}}; P(C) \approx \frac{n_C}{n}$$

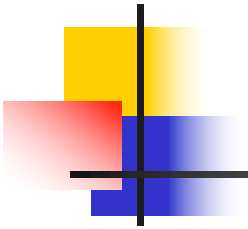
KNN Classification

- Evaluation
  - Performance function:
    - Probability of a data point at x having label l assuming generalization through the chosen kernel function
      - In standard KNN the kernel is a hyperspherical window

$$P(C \mid x) = \frac{p(x \mid C)P(C)}{p(x)} = \frac{\frac{k_C}{n_C V_{h(k)}} \frac{n_C}{n}}{\frac{k}{nV_{h(k)}}} = \frac{k_c}{k}$$

  - Optimization criterion:
    - Maximum Posterior Estimate (MAP) in the spherical region around x containing K data points

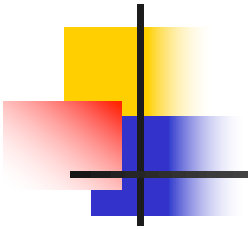
$$\hat{C} = \operatorname{argmax}_C P(C \mid x)$$



KNN Classification

- KNN is a simple algorithm that provides an approximate MAP estimate of the class
  - Makes a number of assumptions
    - Probability density interpolates according to kernel
      - Weighted KNN corresponds to distance-dependent kernels
    - Point estimates are independent
  - Can be extended to regression problems by using weights and estimated value as the output
  - Requires no training time but significant prediction time that grows with the size of the training set

Representation for Classification



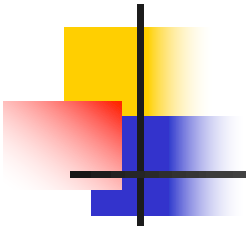
- KNN uses a non-parametric representation to learn MAP classification
  - Representation contains all data pints in the training data set
    - There are ways to reduce this size
- Other, parametric representations can be used for the same problem
  - Simplest representation would be storing the underlying parameters of the MAP problem
    - *P(c), P(x/c)* - Bayesian Learning

Bayesian Classification

- Bayesian classification determines the class with the highest a posteriori (MAP) probability for a given input using the training data set
  - Class is picked as the one with the highest MAP probability

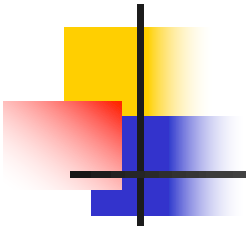
$$\hat{c} = \text{argmax}_c \, P(c \mid x) = \text{argmax}_c \frac{P(x \mid c)P(c)}{P(x)} = \text{argmax}_c \, P(x \mid c)P(c)$$

  - Training data set is used to learn the best parameters for the classifier $P(x \mid c), \quad P(c)$
    - The parameter space is exponential in the number of features x_i in x $\quad x = \langle x_1, \ldots, x_m \rangle$



Bayesian Classification

- Bayesian classification using conditional probabilities as parameters is intractable
  - Number of features grows rapidly
    - Very fast exceeds the amount of memory available
  - Often more parameters than data points
    - Parameters can not be learned well from the data
- To use Bayesian classification, some assumptions have to be made
  - Conditional independence of features given a class



Bayesian Classification

- Conditional independence of some of the features leads to a reduction of the parameter space
  - Partial conditional independence – features are conditionally independent of some other features, but not all of them
    - Bayesian networks
  - Complete conditional independence – all features are conditionally independent given the class
    - Naïve Bayes

Naïve Bayes Classification

- Making the assumption that all features are conditionally independent given the class reduces the number of parameters

$$P(x_i \mid c_i), \quad P(c_i)$$

  - Number of parameters is linear in the number of features
  - MAP parameters can be computed from the smaller set of parameters

$$P(x \mid c) = \prod_i P(x_i \mid c)$$

Naïve Bayes Classification

- Independence reduces the classifier to

$$\hat{c} = \operatorname{argmax}_c P(c \mid x) = \operatorname{argmax}_c P(c) \prod_i P(x_i \mid c)$$

  - Learning requires determining the parameters $P(c_i)$ and $P(x_i/c_i)$ from the data
    - MLE for the parameters can be used

$$P(c_i) = \frac{\#(x^{(j)}, y^{(j)}) \in D : y^{(j)} = c_i}{|D|}$$

$$P(x_i = a \mid c_j) = \frac{\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j \wedge x_i^{(k)} = a}{\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j}$$

Naïve Bayes Classification

- MLE for the parameters has problems
  - Estimation quality deteriorates when there is limited data
    - Many parameters end up 0 or 1
- Can use MAP estimate instead
  - For binary features the answer is the MAP of a Bernoulli distribution with a Beta distribution prior

$$P(x_i = a \mid c_j) = \frac{\left(\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j \wedge x_i^{(k)} = a\right) + \beta_a - 1}{\left(\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j\right) + \beta_a + \beta_{\bar{a}} - 2}$$

Naïve Bayes Classification

- For multinomial features MAP corresponds to a multinomial distribution with its conjugate Dirichlet prior
  - This corresponds to Laplace smoothing
    - For the case where we all β are the same this gives

$$P(c_i) = \frac{\left(\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j\right) + \beta}{|D| + |C|\beta}$$

$$P(x_i = a \mid c_j) = \frac{\left(\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j \wedge x_i^{(k)} = a\right) + \beta}{\left(\#(x^{(k)}, y^{(k)}) \in D : y^{(k)} = c_j\right) + |A|\beta}$$

    - This is equivalent to adding β observations to each count

Naïve Bayes Classification

- Naïve Bayesian classification (and Bayesian classification in general) has additional numeric problems
  - The more features, the smaller the posterior in general
    - More stable to solve Bayesian classification in log likelihood space

$$\hat{c} = \text{argmax}_c \, P(c) \prod_i P(x_i \mid c) = \text{argmax}_c \log\left(P(c) \prod_i P(x_i \mid c) \right)$$

$$= \text{argmax}_c \left(\log P(c) + \sum_i \log P(x_i \mid c) \right)$$

Bayesian Classification

- If features are continuous it is no longer possible to represent all conditional probability density values even under the Naïve Bayes assumption
  - Need to introduce parameters to represent the probability density function of every feature given a class
    - Common choice is a Gaussian distribution

$$p(x_i = z \mid c_j) = N(z \mid \mu_{i,j}, \sigma_{i,j})$$

Gaussian Naïve Bayes

- Naïve Bayes criterion stays the same

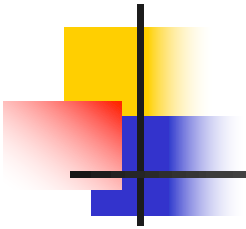
$$\hat{c} = \text{argmax}_c \, P(c \mid x) = \text{argmax}_c \, P(c) \prod_i p(x_i \mid c)$$

  - Need to learn the Gaussian parameters from data
    - Using MLE the expected mean of the Gaussian Gaussian is the expected value in the data

$$\hat{\mu}_{i,j} = E[x_i \mid c_j] = \frac{\sum_{k:y^{(k)}=c_j} x_i^{(k)}}{\#(x^{(k)}, y^{(k)}) : y^{(k)} = c_j}$$

    - Similarly the expected variance is the unbiased variance of the data in the class

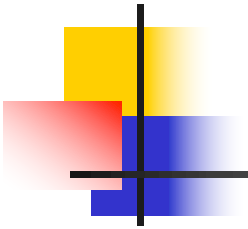
$$\hat{\sigma}_{i,j}^2 = \frac{\sum_{k:y^{(k)}=c_j} (x_i^{(k)} - \mu_{i,j})^2}{\left(\#(x^{(k)}, y^{(k)}) : y^{(k)} = c_j\right) - 1}$$



Naïve Bayes Classification

- Naïve Bayes is a commonly applied technique for probabilistic classification
  - Naïve Bayes is usually relatively easy to apply
  - Uses relatively intuitive parameters
  - Number of parameters is linear in the number of features
  - Often yields good results
  - Independence assumption is usually not strictly correct
  - Requires significant data to estimate its parameters
  - Makes relatively limiting assumptions for continuous features

Generative vs. Discriminative Learners



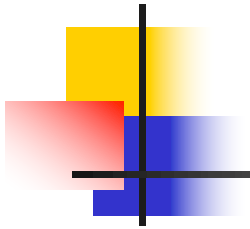
- Supervised learning algorithms are often divided into two groups
  - Generative algorithms
  - Discriminative algorithms
- Generative algorithms are algorithms that learn a model for the process that generates the data and use this to predict the output
- Discriminative algorithms directly learn to predict/discriminate the output

Generative vs. Discriminative Learners

- Generative algorithms allow to predict the output and to generate simulated data
  - Learn $p(x \mid y)$ and potentially $p(y)$
  - Use MLE or MAP to predict the output

- Discriminative algorithms directly learn to predict/discriminate the output
  - Learn $p(y \mid x)$ or directly the MAP estimate for y

Generative vs. Discriminative Learners



- Both types of learners have their advantages and disadvantages
  - Generative algorithms can be used to produce simulated data
  - Parameters for generative algorithms are often easier to extract from the data
  - Discriminative algorithms often have more compact representations (particularly if they directly learn to predict the MAP estimate)