Alpaydin’s Introduction to Machine Learning

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Contents

Supervised Learning

Vapnik-Chervonenkis Dimension

- Given a dataset containing N points, a hypothesis H shatters N points if it separates the positive examples from the negative.
- **Vapnik-Chervonenkis (VC) dimension** of a hypothesis H, denoted as $\mathrm{VC}(H)$: The maximum number of points that can be shattered by H.

Probably Approximately Correct Learning

- Given a class C, and examples drawn from some unknown but fixed probability distribution $p(x)$.
- We want to find the number of examples, N, such that with probability at least $1 - \delta$, the hypothesis H has error at most ε, for arbitrary $\delta \leq \frac{1}{2}$ and $\varepsilon > 0$,.
- $P(C\Delta H \leq \varepsilon) \geq 1 - \delta$, where $C\Delta H$ is the region of difference between C and H.

Noise

- Noise can result from:
    - Imprecision in recording the input attributes.
    - Errors in labeling the data points.
    - Hidden or latent attributes that may be unobservable.
- **Occam's razor**: simpler explanations are more plausible and any unnecessary complexity should be shaved off.

Regression

- If there is no noise, the task is *interpolation/extrapolation*.
- In regression, there is noise added to the output of the unknown function.

Model Selection and Generalization

- An **ill-posed problem** is where the data by itself is not sufficient to find a unique solution.
- **Model selection**: Choosing between possible hypothesis.
- **Generalization**: How well a model trained on the training set predicts the right output for new instances.
- **Triple trade-off**:
    - The complexity of the hypothesis we fit to data.
    - The amount of training data.
    - The generalization error on new examples.
- In general, as the complexity of a model class increases, the generalization error decreases first and then starts to increase.
- Datasets:
    - **Training set**: To train the model.
    - **Validation set**: To test the generalization ability.

  - **Test set**, or **publication set**: To report the error to give an idea about the expected error of our best model.
- In *cross-validation*, the hypothesis that is the most accurate on the validation set is the best one.

Dimensions of a Supervised Machine Learning Algorithm

- There are three decisions we must make:
  - **Model**: Denoted as $\hat{f}(x|\theta)$ where $\hat{f}$ is the model, x is the input, and θ are the parameters.
  - **Loss function** (L): To compute the difference between the desired output and our approximation to it.
  - **Optimization procedure**: To find θ^* that minimizes the total error.

Bayesian Decision Theory

- Introduction
- Classification
- Losses and Risks
- Discriminant Functions
- Association Rules
- Notes

Classification

- **Bayes' rule**: $P(y=i|x)$ = $P(y=i)P(x|y=i)/P(x)$ where
  - $P(y=i|x)$ is the **posterior probability**.
  - $P(y=i)$ is the **prior probability**.
  - $P(x|y=i)$ is the **likelihood**.
  - $P(x)$ is the **evidence**.
- **Bayes' classifier**: Given an observation x, the predicted class $\hat{y}$ = $\text{argmax}_i P(y=i|x)$.

Losses and Risks

- Let λ_{ik} be the loss incurred for falsely assuming $\hat{y}$ = i when the input actually belongs to y = k.
- The *expected loss* for misclassification is $L(y=i|x)$ = $\sum_{k=1}^{K} \lambda_{ik} P(y=k|x)$.
- The class with the least expected loss is $\text{argmin}_i L(y=i|x)$.
- In Bayesian classifier, λ_{ik} is 0 if i = k, or 1 if $i \neq k$.

- $\hat{y}$ = $\text{argmin}_i L(y=i|x)$ = $\text{argmin}_i \sum_{k=1}^{K} \lambda_{ik} P(y=k|x)$ = $\text{argmin}_i 1 - P(y=i|x)$ = $\text{argmax}_i P(y=i|x)$.

Discriminant Functions

- Classification can be seen as implementing a set of *discriminant functions*, $g_i(x), i \in \{1, \ldots, K\}$, such that $\hat{y}$ = $\text{argmax}_i g_i(x)$.
- This divides the feature space into K *decision regions* $R_i, i \in \{1, \ldots, K\}$.
- The regions are separated by *decision boundaries*.

Association Rules

- An association rule is an implication of the form $X \rightarrow Y$ where X is the **antecedent** and Y is the **consequent** of the rule.
- **Support**: support$(X \rightarrow Y)$:= $P(X, Y)$.
- **Confidence**: confidence$(X \rightarrow Y)$:= $P(Y|X)$.
- **Lift** (or **interest**): lift$(X \rightarrow Y)$:= $\frac{P(X,Y)}{P(X)P(Y)}$ = $\frac{P(Y|X)}{P(Y)}$.
- Two steps of **Apriori** algorithm:
  1. Find frequent item sets, that is, those which have enough *support*.
  2. Convert them to rules with enough *confidence* by splitting the items into two, as items in the *antecedent* and items in the *consequent*.
- A rule $X \rightarrow Y$ need not imply causality but just an association.
- In a problem, there may also be *hidden variables* whose values are never known through evidence.

Parametric Methods

Maximum Likelihood Estimation

- Let $X = \{x_i\}_{i=1}^N$ be a set of N independent and identically distributed (iid) samples drawn from some known probability density family.
- The **likelihood** of parameter θ given sample X is the product of the likelihoods of the individual points: $I(\theta|X) = P(X|\theta) = \prod_{i=1}^N P(x_i|\theta)$.
- **Log likelihood**: $L(\theta|X) = \log I(\theta|X) = \log P(X|\theta) = \sum_{i=1}^N P(x_i|\theta)$.
- **Maximum likelihood estimation (MLE)**: $\hat{\theta} = \text{argmax}_\theta I(\theta|X) = \text{argmax}_\theta L(\theta|X)$.
- **Bernoulli density**:
  - $X \sim B(N, \theta)$.
  - $P(x_i|\theta) = \theta^{xi}(1-\theta)^{1-xi}$.
  - $L(\theta|X) = \log \prod_{i=1}^N \theta^{xi}(1-\theta)^{1-xi} = \sum_i x_i \log\theta + (N - \sum_i x_i)\log(1-\theta)$.
  - $\hat{\theta} = \sum_i x_i/N$.
- **Multinomial density**:
  - $X \sim \text{multinomial}(N, \theta)$, where $\theta = \{\theta_i | i = 1, \ldots, K\}$.
  - $P(x_i|\theta) = \prod_{k=1}^K \theta_i^{xik}$ where x_{ik} is 1 if $x_i = k$, or 0 if $x_i \neq k$.
  - $\hat{\theta}_k = \sum_i x_{ik}/N$, $k \in \{1, \ldots, K\}$.
- **Gaussian density**:
  - $X \sim N(\mu, \sigma^2)$.
  - $P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\text{exp}(-\frac{(xi-\mu)^2}{2\sigma^2})$.
  - $\hat{\mu} = \sum_i x_i/N$.
  - $\hat{\sigma^2} = \sum_i (x_i - \hat{\mu})^2/N$.

Evaluating an Estimator: Bias and Variance

- Let $\hat{\theta}$ be an estimator of θ based on N observations.
- **Bias** of an estimator: $b_\theta(\hat{\theta}) := E[\theta - \hat{\theta}]$.
- **Mean square error (MSE)** of an estimator: $r_\theta(\hat{\theta}) := E[(\theta - \hat{\theta})^2]$.
- **Unbiased estimator**: $\hat{\theta}$ is an *unbiased* estimator of θ if $b_\theta(\hat{\theta}) = 0$ or $E[\hat{\theta}] = \theta$.
- **Consistent estimator**: $\hat{\theta}$ is a *consistent* estimator of θ if $r_\theta(\hat{\theta}) \to 0$ as $N \to 0$.
- $m = \sum_i x_i/N$ is an unbiased and consistent estimator of μ.
- $s^2 = \sum (x_i - m)^2/N$ is a biased but consistent estimator of σ^2 since $E[s^2] = \frac{N-1}{N}\sigma^2 \neq \sigma^2$.
- **Asymptotically unbiased estimator**: $\hat{\theta}$ is an *asymptotically unbiased* estimator of θ if $b_\theta(\hat{\theta}) \to 0$ or $E[\hat{\theta}] \to \theta$ as $N \to 0$.
- MSE = $r_\theta(\hat{\theta}) = b_\theta^2(\hat{\theta}) + \text{variance}(\hat{\theta})$ = bias^2 + variance.

The Bayes' Estimator

- The estimation of θ can be exploited by prior information on the distribution of θ.
- **Bayes' rule**: $P(\theta|X) = P(\theta)P(X|\theta)/P(X)$ where
    - **Posterior density** $P(\theta|X)$: the likely θ values after looking at the sample.
    - **Prior density** $P(\theta)$: the likely values that θ may take before looking at the sample.
- **Maximum likelihood estimate (MLE)**: $\hat{\theta} = \text{argmax}_{\theta} P(X|\theta)$.
- **Maximum a posteriori (MAP) estimate**: $\hat{\theta} = \text{argmax}_{\theta} P(\theta|X)$.
- **Bayes' estimate**: $\hat{\theta} = E[\theta|X] = \int \theta P(\theta|X) d\theta$.
- The Bayes' estimator for posterior mean $\hat{\mu}$ is a weighted average of the prior mean μ and the sample mean m.

Parametric Classification

- In *Bayes' classification*, the discriminant function for class $i \in \{1, \ldots, K\}$ is
  - $g_i(x) = P(x|y=i)P(y=i)$
  - $g_i(x) = \log P(x|y=i) + \log P(y=i)$.
- **Gaussian Bayes' classification**:
    - Assume $P(x|y=i) \sim N(\mu_i, \sigma_i^2)$.
    - $g_i(x) = -\frac{1}{2}\log 2\pi - \log \sigma_i - \frac{(x-\mu_i)^2}{2\sigma_i^2} + \log P(y=i)$.
    - $\mu_i \sim m_i$ and $\sigma_i^2 \sim s_i^2$ are estimated from N observations using maximum likelihood estimation.
- Simplified *Gaussian Bayes' classification*:
    - Assumption(s):
        - Equal variances, i.e., $\sigma^2 = \sigma_i^2$ for class $i \in \{1, \ldots, K\}$.
        - Equal priors, i.e., $P = P(y=i)$ for class $i \in \{1, \ldots, K\}$.
    - $g_i(x) \propto -\frac{(x-m_i)^2}{2s_i^2}$ and $\text{argmax}_i g_i(x) = \text{argmin}_i |x - m_i|$if
    - The decision boundary is the midpoint between the two means.

Regression

- $y = f(x) + \varepsilon$: The numeric output is the sum of a deterministic function of the input and random noise.
- $f(x)$, the unknown function, is approximated by the estimator $\hat{f}(x|\theta)$.
- Assume that ε is zero mean Gaussian with constant variance σ^2, namely, $\varepsilon \sim N(0, \sigma^2)$.
- By placing $\hat{f}(x|\theta)$ in place of $f(x)$, we have $P(y|x) \sim N(\hat{f}(x|\theta), \sigma^2)$.
- $P(x, y) = P(y|x)P(x)$, where $P(y|x)$ is the output given the input, and $P(x)$ is the input density.
- $L(\theta|X) = \log \prod_{i=1}^{N} P(x_i, y_i) = \log \prod_{i=1}^{N} P(y_i|x_i) + \log \prod_{i=1}^{N} P(x_i)$.
- **Linear regression**:

- Assume Gaussian distributed error.
- Maximizing likelihood corresponds to minimizing the sum of squared errors.
- $\hat{f}(x|w_0, w_1) = w_0 + w_1x$.
- $\text{argmax}_{w0,w1}L(w_0, w_1|X) = \text{argmax}_{w0,w1} \log \prod_{i=1}^{N} P(y_i|x_i) = \text{argmax}_{w0,w1} \sum_{i=1}^{N}(y_i - \hat{f}(x_i|w_0, w_1))^2$.

- **Relative squared error (RSE)**: RSE = residual sum of squares (RSS) / total sum of squares (TSS) = $\sum_i(y_i - \hat{y}_i)^2 / \sum_i(y_i - \bar{y})^2$.
- **Coefficient of determination**: R^2 = 1 - RSE.

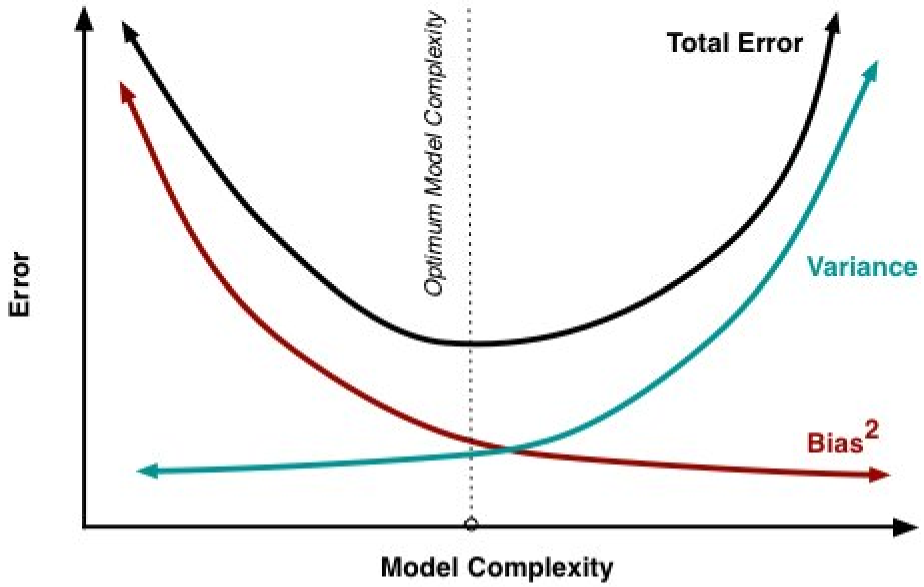
Tuning Model Complexity: Bias/Variance Dilemma

- Consider $y = f(x) + \varepsilon$, where $\varepsilon \sim N(0, \sigma^2)$ and $\hat{f}$ is an estimator of f.
- **Mean squared error (MSE)** of a model: $E[(y - \hat{f})^2] = E[(f - \hat{f} + \varepsilon)^2] = E[(f - \hat{f})^2] + 2E[(f - \hat{f})\varepsilon] + E[\varepsilon^2] = E[(f - \hat{f})^2] + E[\varepsilon^2] = b_f(\hat{f})^2 + r_f(\hat{f}) + \sigma^2$ = bias^2 + variance + noise.
- **Bias/variance dilemma**: Models with a lower bias in parameter estimation have a higher variance of the parameter estimates across samples, and vice versa.
- In a sense, high bias implies **underfitting** and high variance implies **overfitting**.

Model Selection Procedures

- In practice, we cannot calculate the bias and variance for a model, but we can calculate the total error.
- **Cross-validation**:
  - The validation error is an estimate of the total error except that it also contains the variance of the noise.
  - Cross-validation makes no prior assumption about the model or parameters.
- **Regularization** introduce an **augmented error function** to penalizes complex models with large variance.
- The augmented error function can be seen as an **optimism** estimating the discrepancy between training and test error.
- The weight of the penalty λ is optimized using cross-validation.
- **Akaike's information criterion (AIC)** and **Bayesian information criterion (BIC)** work by estimating the optimism and adding it to the training error to estimate test error, without any need for validation.
- **Structural risk minimization (SRM)** uses a set of models ordered in terms of their complexities.
- **Minimum description length (MDL)** is based on an information theoretic measure.

- **Bayesian model selection** is used when we have some prior knowledge about the appropriate class of approximating functions.



Multivariate Methods

- Multivariate Data
- Parameter Estimation
- Estimation of Missing Values
- Multivariate Normal Distribution
- Multivariate Classification
- Tuning Complexity
- Discrete Features
- Multivariate Regression

Estimation of Missing Values

- **Imputation**: the process of replacing missing data with substituted values.
  - **Mean imputation** substitutes the mean (average) of the available data for that variable in the sample.
  - **Imputation by regression** predicts the value of a missing variable from other variables whose values are known for that case.

Multivariate Normal Distribution

- **Mahalanobis distance**: $(x-\mu)^\top \Sigma^{-1}(x-\mu)$.

- The projection of a d-dimensional normal on the vector w is univariate normal.
- Suppose $x\ N(\mu, \Sigma)$. Then, $w^\top x\ N(w^\top \mu, w^\top \Sigma w)$.

Multivariate Classification

- Assume that the feature space is D-dimensional.
- The discriminant function for class $i \in \{1, \ldots, K\}$: $g_i(x) = \log P(x|y = i) + \log P(y = i)$.
- Assume $P(x|y = i) \sim N(\mu_i, \Sigma_i)$.
- $g_i(x) = -\frac{D}{2} \log 2\pi - \frac{1}{2} \log |\Sigma_i| - \frac{1}{2}(x - \mu_i)^\top \Sigma_i^{-1}(x - \mu_i) + \log P(y = i)$.
- $\mu_i \sim m_i$ and $\Sigma_i \sim S_i$ are estimated from N observations using maximum likelihood estimation.
- **Quadratic discriminant analysis (QDA)**:
  - $g_i(x) \propto x^\top W_i x + w_i^\top x + b_i$, where
    - $W_i = -\frac{1}{2} S_i^{-1}$.
    - $w_i = S_i^{-1} m_i$.
    - $b_i = -\frac{1}{2} \log |S_i| - \frac{1}{2} m_i^\top + \log \hat{P}(y = i)$.
  - The decision boundary is a quadric hypersurface in D-dimensional space.
  - The number of parameters:
    - KD for the means.
    - $KD(D + 1)/2$ for the covariance matrices.
- **Linear discriminant analysis (LDA)**:
  - Assumption(s):
    - Covariance matrix for each class is shared, i.e., $\Sigma = \Sigma_i$ for class $i \in \{1, \ldots, K\}$.
  - $g_i(x) \propto w_i^\top x + b_i$, where
    - $w_i = S^{-1} m_i$.
    - $b_i = -\frac{1}{2} m_i^\top S^{-1} m_i + \log \hat{P}(y = i)$.
  - The number of parameters:
    - KD for the means.
    - $D(D + 1)/2$ for the shared covariance matrix.
- **Naive Bayes' classifier**:
  - Assumption(s):
    - Covariance matrix for each class is shared, i.e., $\Sigma = \Sigma_i$ for class $i \in \{1, \ldots, K\}$.
    - Independent variables, i.e., Σ is diagnoal.
  - The number of parameters:
    - KD for the means.
    - D for the shared variances.
- **Euclidean distance classifier**:
  - Assumption(s):
    - Covariance matrix for each class is shared, i.e., $\Sigma = \Sigma_i$ for class $i \in \{1, \ldots, K\}$.

    - Independent variables, i.e., Σ is diagnoal.
    - Equal variances, i.e., $\Sigma = \sigma^2 I$.
  - The number of parameters
    - KD for the means.
    - 1 for the shared variance.
- **Nearest centroid classifier**:
  - Assumption(s):
    - Covariance matrix for each class is shared, i.e., $\Sigma = \Sigma_i$ for class $i \in \{1, \dots, K\}$.
    - Independent variables, i.e., Σ is diagnoal.
    - Equal variances, i.e., $\Sigma = \sigma^2 I$.
    - Equal priors, i.e., $P = P(y = i)$ for class $i \in \{1, \dots, K\}$.
  - The number of parameters:
    - KD for the means.
    - 1 for the shared variance.

Tuning Complexity

- **Regularized discriminant analysis (RDA)**:
  - Substitute covariance matrix for class S_i' is the sum of three weighted components:
    - $\alpha s^2 I$: identity matrix.
    - βS: shared covariance matrix.
    - $(1 - \alpha - \beta) S_i$: class-specific covariance matrix.
  - Consider three scenarios:
    - $\alpha = \beta = 0$: quadratic discriminant analysis (QDA).
    - $\alpha = 0$ and $\beta = 1$: linear discriminant analysis (LDA).
    - $\alpha = 1$ and $\beta = 0$: nearest centroid classifier.
  - α and β are optimized by cross-validation.

Dimensionality Reduction

Introduction

- The complexity depends on the number of input dimensions.
- Two main methods for reducing dimensionality:
    - **Feature selection**: finding k of the d dimensions.
    - **Feature extraction**: finding a new set of k dimensions that are combinations of the original d dimensions.
- Categories of *feature extraction* methods:
    - *Unsupervised*:
        - *Linear*: principal component analysis, factor analysis, multidimensional scaling
        - *Nonlinear*: isometric feature mapping, locally linear embedding, Laplacian eigenmaps
    - *Supervised*: linear discriminant analysis,

Subset Selection

- Two approaches: **forward selection** vs **backward selection**.
- Subset selection is *supervised*.

Principal Component Analysis

- Given data x_1, ..., x_n, with $\mathrm{Cov}(x) = \Sigma$.
- PCA is an optimization problem that maximizes the variance of the projection of x on the direction of w, where w is a unit vector.
- Mathematical definition: maximize $\mathrm{Var}(w^\top x) = w^\top \mathrm{Cov}(x) w = w^\top \Sigma w$ subject to $w^\top w = 1$.
- Lagrange problem: maximize $w^\top \Sigma w - \lambda(w^\top w - 1)$.
- Taking the derivative with respect to w and setting it equal to 0, we have $\Sigma w = \lambda w$.
- The principal component is the eigenvector of the covariance matrix with the largest eigenvalue.
- **Spectral decomposition**: Let S be a symmetric matrix. $S = W \lambda W^{-1} = W \lambda W^\top$.
- **Proportion of variance** explained by the k principal components is $\sum_{i=1}^{k} \lambda_i / \sum_{i=1}^{d} \lambda_i$.
- **Scree graph**: the plot of explained variance as a function of the number of eigenvectors kept.
- **Karhunen-Loève expansion** allows using class information.
- **Common principal components** assumes:
    - The principal components are the same for each class.
    - The variances of these components differ for different classes.

Feature Embedding

- X is the $N \times d$ data matrix that has zero mean in each input dimension (column).

- **Feature embedding**: the N-dimensional eigenvectors of $XX^\top$ are the coordinates in the new space.
- Feature embedding does not fit a projection model as PCA does. Instead, it gets the coordinates directly.
- $XX^\top$ can be considered as an $N \times N$ matrix of pairwise similarities.
- Feature embedding respects the original pairwise similarities.