Machine Learning
Theory

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Abstract

The course topics are:

- Introduction: basic concepts.
- Learning theory:
  - Bias/variance tradeoff. Union and Chernoff/Hoeffding bounds.
  - VC dimension. Worst case (online) learning.
  - Practical advice on how to use learning algorithms.
- Supervised learning:
  - Supervised learning setup. LMS.
  - Logistic regression. Perceptron. Exponential family.
  - Kernel methods: Radial Basis Networks, Gaussian Processes, and Support Vector Machines.
  - Model selection and feature selection.
  - Ensemble methods: Bagging, boosting.
  - Evaluating and debugging learning algorithms.
- Reinforcement learning and control:
  - MDPs. Bellman equations.
  - Value iteration and policy iteration.
  - TD, SARSA, Q-learning.
  - Value function approximation.
  - Policy search. Reinforce. POMDPs.
  - Multi-Armed Bandit.

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CHAPTER 1

Introduction

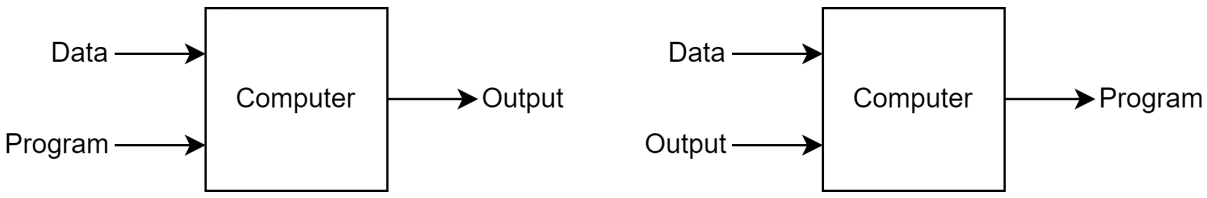
1.1 Machine learning

Definition (*Learning*)**.** A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, improves with experience E.

Machine learning, a subset of artificial intelligence, derives knowledge from experience and induction.

In machine learning, we depend on computers to make informed decisions using new, unfamiliar data. Designing a comprehensive set of meaningful rules can prove to be exceedingly difficult. Machine learning facilitates the automatic extraction of relevant insights from historical data and effectively applies them to new datasets.

The objective is to automate the programming process for computers, acknowledging the bottleneck presented by writing software. Instead, our aim is to utilize the data itself to accomplish the required tasks.



(a) Programming (b) Machine learning

Figure 1.1: Difference between programming and machine learning

Machine learning paradigms can be categorized into three main types:

- *Supervised learning*: involves labeled data and direct feedback, aiming to predict outcomes or future events.
- *Unsupervised learning*: operates without labeled data or feedback, focusing on discovering hidden structures within the data.
- *Reinforcement learning*: centers around a decision-making process, incorporating a reward system to learn sequences of actions.

1.1.1 Supervised learning

Supervised learning encompasses several distinct tasks:

- *Classification*: this involves assigning predefined categories or labels to data points based on their features. The model is trained on labeled data, learning patterns to predict the class labels of new data points.
- *Regression*: the goal here is to predict continuous numerical values based on input features, as opposed to discrete class labels in classification. The model learns a function mapping input features to output values.
- *Probability estimation*: this task predicts the likelihood of certain events or outcomes occurring, often used to gauge the confidence of model predictions.

Formally, in supervised learning, a model learns from data to map known inputs to known outputs. The training set is denoted as $\mathcal{D} = \{\langle x, t\rangle\}$, Where $t = f(x)$, with f representing the unknown function to be determined using supervised learning techniques.

Various techniques can be employed for supervised learning, including linear models, artificial neural networks, support vector machines, and decision trees.

1.1.2 Unsupervised learning

Unsupervised learning encompasses two main tasks:

- *Clustering*: in this task, the objective is to group similar data points together based on their features, without predefined labels. The goal is to uncover underlying patterns or structures within the data. Clustering algorithms segment the data into clusters or groups, where data points within the same cluster exhibit greater similarity compared to those in different clusters. Unlike supervised learning, where labeled data is provided, clustering algorithms explore data solely based on features to identify similarities.
- *Dimensionality reduction*: this task involves reducing the number of input variables or features in a dataset while retaining essential information. This is often done to address the curse of dimensionality, enhance computational efficiency, and mitigate overfitting risks in models. Dimensionality reduction techniques aim to transform high-dimensional data into a lower-dimensional representation while preserving most relevant information.

Formally, in unsupervised learning, computers learn previously unknown patterns and efficient data representations. The training set is defined as $\mathcal{D} = \{x\}$, where the goal is to find a function f that extracts a representation or grouping of the data.

Various techniques are used for unsupervised learning, including k-means clustering, self-organizing maps, and principal component analysis.

1.1.3 Reinforcement learning

Reinforcement learning encompasses several key approaches:

- *Markov decision process*: a mathematical framework for modeling decision-making, involving states, actions, transition probabilities, and rewards. The goal is to find a policy that maximizes cumulative rewards while considering uncertainty.

- *Partially observable MDP*: an extension of MDP where the current state is uncertain and must be inferred from observations. The objective remains the same, but the agent maintains a belief over possible states based on observations.
- *Stochastic games*: models for decision-making with multiple agents, where outcomes depend on actions and random factors. Players aim to optimize strategies considering other players' actions and uncertainties.

In reinforcement learning, the computer learns the optimal policy based on a training set $\mathcal{D}$ containing tuples $\langle x, u, x', r \rangle$, where x is the input, u is the action, x' is the resulting state after the action, and r is the reward. The policy Q^* is defined to maximize $Q^*(x, u)$ over actions u for each state x in the training set.

Various techniques such as Q-learning, SARSA, and fitted Q-iteration are used to find this optimal policy.

CHAPTER 2

Supervised learning

2.1 Introduction

Supervised learning stands as the predominant and well-established learning approach. Its core objective is to enable a computer, given a training set $\mathcal{D} = \{\langle x, t \rangle\}$, to approximate a function f that maps an input x to an output t. The input variables x, often referred to as features or attributes, are paired with output variables t, also known as targets or labels. The tasks undertaken in supervised learning are as follows:

- *Classification*: when t is discrete.
- *Regression*: when t is continuous.
- *Probability estimation*: when$t$ represents a probability.

Supervised learning finds application in scenarios where:

- Humans lack the capability to perform the task directly (e.g., DNA analysis).
- Humans can perform the task but lack the ability to articulate the process (e.g., medical image analysis).
- The task is subject to temporal variations (e.g., stock price prediction).
- The task demands personalization (e.g., movie recommendation).

2.1.1 Function approximation

The process of approximating a function f from a dataset $\mathcal{D}$ involves several steps:

1. *Define a loss function* $\mathcal{L}$: this function calculates the discrepancy between f and h, a chosen approximation.
2. *Select a hypothesis space* $\mathcal{H}$: this space consists of a set of candidate functions from which to choose an approximation h.
3. *Minimize* $\mathcal{L}$ *within* $\mathcal{H}$: the goal is to find an approximation h within the hypothesis space $\mathcal{H}$ that minimizes the loss function $\mathcal{L}$.

The hypothesis space $\mathcal{H}$ can be expanded to theoretically achieve a perfect approximation of the function f. However, a significant challenge arises because the loss function $\mathcal{L}$ cannot be easily determined, primarily due to the absence of the actual function f.

2.1.2 Taxonomy

The taxonomy is as follows:

- *Parametric* or *nonparametric*: parametric methods are characterized by having a fixed and finite number of parameters, while nonparametric methods have a number of parameters that depend on the training set.
- *Frequentist* or *Bayesian*: frequentist approaches utilize probabilities to model the sampling process, whereas Bayesian methods use probability to represent uncertainty about the estimate.
- *Empirical risk minimization* or *structural risk minimization*: empirical risk refers to the error over the training set, while structural risk involves balancing the training error with model complexity.

The type of machine learning can be:

- *Direct*: This method involves learning an approximation of f directly from the dataset $\mathcal{D}$.
- *Generative*: in this approach, the model focuses on modeling the conditional density $\mathrm{P}(t|x)$ and then marginalizing to find the conditional mean:

$$\mathbb{E}\left[t|x\right] = \int t \cdot \mathrm{P}(t|x)dt$$

- *Discriminative*: This method models the joint density $\mathrm{P}(x,t)$, infers the conditional density $\mathrm{P}(t|x)$, and then marginalizes to find the conditional mean:

$$\mathbb{E}\left[t|x\right] = \int t \cdot \mathrm{P}(t|x)dt$$

2.2 Linear regression

The goal of regression is to approximate a function $f(x)$ that maps input x to a continuous output t from a dataset $\mathcal{D}$:

$$\mathcal{D} = \{\langle x, t\rangle\} \implies t = f(x)$$

Here, x is a vector. To perform regression, we assume the existence of a function capable of performing this mapping. The key components of constructing a linear regression problem include:

- The method used to model the function f (the hypothesis space).
- The evaluation criteria for the approximation (the loss function).
- The optimization process for optimizing the model.

In linear regression, the function f is modeled using linear functions. This choice is motivated by several factors:

- Linear models are easily interpretable, making them suitable for explanation.
- Linear regression problems can be solved analytically, allowing for efficient computation.
- Linear functions can be extended to model nonlinear relationships.
- More sophisticated methods often build upon or incorporate elements of linear regression.

Hypothesis space In mathematical terms, the approximation y can be defined as:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{D-1} w_j x_j = \mathbf{w}^T \mathbf{x}$$

Here, $\mathbf{x} = (1, x_1, \ldots, x_{D-1})$ is a vector, and w_0 is called the bias parameter. It's important to note that the output y is a scalar value.

In a two-dimensional space, our hypothesis space will be the set of all points in the plane (w_0, w_1). The coordinates of each point will correspond to a line in the $(\mathbf{x}, y)$ space.

Loss function A commonly used error loss function for the linear regression problem is the sum of squared errors (SSE), defined as:

$$L(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \left(y(x_n, \mathbf{w}) - t_n\right)^2$$

This sum is also referred to as the residual sum of squares (RSS) and can be expressed as the sum of squared residual errors:

$$RSS(\mathbf{w}) = \left\|\boldsymbol{\epsilon}_2^2\right\| = \sum_{i=1}^{N} \epsilon_i^2$$

This formulation of the loss function allows for obtaining a closed-form optimization solution.

Optimization For linear models, a closed-form optimization of the RSS, known as least squares, begins with the matrix representation of the loss function:

$$L(\mathbf{w}) = \frac{1}{2} RSS(\mathbf{w}) = \frac{1}{2} \left(\mathbf{t} - \boldsymbol{\Phi}_{\mathbf{w}}\right)^T \left(\mathbf{t} - \boldsymbol{\Phi}_{\mathbf{w}}\right)$$

Here, $\boldsymbol{\Phi} = \begin{bmatrix}\phi(x_1) & \ldots & \phi(x_N)\end{bmatrix}^T$ and $\mathbf{t} = \begin{bmatrix}t_1 & \ldots & t_n\end{bmatrix}^T$. To find the optimal $\mathbf{w}$, we compute the first derivative of $L(\mathbf{w})$ and set it to zero:

$$\hat{\mathbf{w}}_{OLS} = \left(\boldsymbol{\Phi}^T \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^T \mathbf{t}$$

However, the inversion of the matrix $\boldsymbol{\Phi}^T \boldsymbol{\Phi}^{-1}$ can be computationally expensive, especially for large datasets, with a complexity of $O(nm^2 + m^3)$, assuming the matrix is non-singular (invertible).

To mitigate this, stochastic gradient descent (SGD) can be employed. The algorithm known as least mean squares (LMS) uses the following update rule:

$$L(\mathbf{x}) = \sum_n L(x_n)$$

Expanding this, we get:

$$\begin{aligned}\mathbf{w}^{(n+1)} &= \mathbf{w}^{(n)} - \alpha^{(n)} \nabla L(x_n) \\ &= \mathbf{w}^{(n)} - \alpha^{(n)} \left(\mathbf{w}^{(n)^T} \phi(\mathbf{x}_n) - t_n \right) \phi(\mathbf{x}_n)\end{aligned}$$

Here, α is the learning rate, and convergence is guaranteed if $\sum_{n=0}^{\infty} = +\infty$ and $\sum_{n=0}^{\infty} = \alpha^{(n)^2} < +\infty$.

If the regression problem involves multiple outputs, meaning that $\mathbf{t}$ is not a scalar, we can solve each regression problem independently. However, we can still use the same set of basis functions. The solution for the weight vectors for all outputs can be expressed as:

$$\hat{\mathbf{W}} = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{T}$$

Here, each column of matrix $\mathbf{T}$ and $\hat{\mathbf{W}}$ corresponds to the target vector and the weight vector for each output, respectively. This solution can be easily decoupled for each output k:

$$\hat{\mathbf{w}}_k = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{t}_k$$

An advantage of this approach is that $\left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1}$ only needs to be computed once, regardless of the number of outputs.

2.2.1 Basis function

While a linear combination of input variables may not always suffice to model data, we can still construct a regression model that is linear in its parameters. This can be achieved by defining a model using non-linear basis functions, expressed as:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

Here, the components of the vector $\boldsymbol{\phi}(\mathbf{x}) = (1, \phi_1(\mathbf{x}), \ldots, \phi_{M-1}(\mathbf{x}))^T$ are referred to as features. These features allow for a more flexible representation of the input data, enabling the model to capture non-linear relationships between the input variables and the output.

Example:
Let's reconsider a set of data regarding individuals' weight and height, along with their completion times for a one-kilometer run:

Height (cm)	Weight (kg)	Completion time (s)
180	70	180
184	80	220
174	60	170

We can model this problem using a dummy variable and introduce the Body Mass Index (BMI) as a new feature:

Dummy variable	**Height (cm)**	**Weight (kg)**	**BMI**	**Completion time (s)**
x_0	x_1	x_2	x_3	t
1	180	70	21	180
1	184	80	23	220
1	174	60	20	170

Here, the dummy variable x_0 is always initialized to one. Now, we have the option to retain or discard the weight and height variables, considering only the BMI values for analysis.

The most commonly used basis functions in regression are:

- *Polynomial*:
$$\phi_j(x) = x^j$$
- *Gaussian*:
$$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2\sigma^2}\right)$$
- *Sigmoidal*:
$$\phi_j(x) = \frac{1}{1+\exp\left(\frac{\mu_j - x}{\sigma}\right)}$$

Here, the constant μ_j is referred to as a hyperparameter, as its value needs to be determined through experimentation and depends on the user's experience.

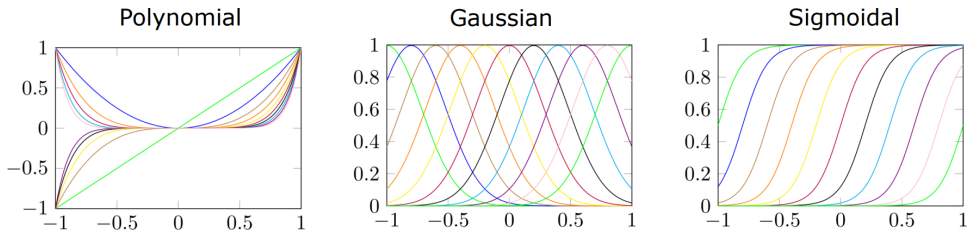


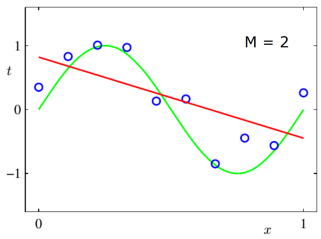
Figure 2.1: Some possible basis functions shapes

It's noteworthy that the Gaussian basis function allows for a local approximation by omitting values that are close to zero. This approach enables capturing the relationship between the input and output in a reduced input space area. As we move away from the mean, approaching zero, the values become negligible.

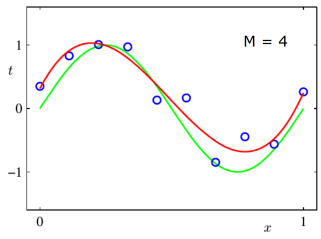
2.2.2 Regularization

A function can achieve a better approximation by increasing the degree of the polynomial used in the regression.

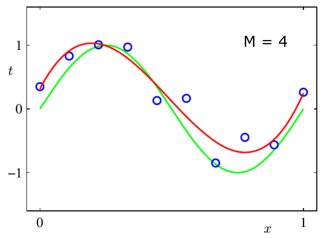
Example:
Consider a function generating a set of points with some noise:



Using a second-order polynomial instead of a linear one provides a better approximation:



Further improving the approximation can be achieved with a higher-degree polynomial (e.g., ninth grade):



However, increasing the polynomial degree also increases the complexity of the model parameters. To address this complexity, adjustments are needed in the loss function:

$$L(\mathbf{w}) = L_D(\mathbf{w}) + \lambda L_W(\mathbf{w})$$

Here, $L_D(\mathbf{w})$ represents the usual loss function, $L_W(\mathbf{w})$ reflects model complexity (a hyperparameter), and λ is the regularization coefficient. $L_W(\mathbf{w})$ can be tailored using ridge regression or lasso methods.

Ridge regression In ridge regression, the regularization term $L_W(\mathbf{w})$ is defined as:

$$L_W(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} = \frac{1}{2}\left\|\mathbf{w}\right\|_2^2$$

Thus, the overall loss function becomes:

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\left(t_i - \mathbf{w}^T\phi(x_i)\right)^2 + \frac{\lambda}{2}\left\|\mathbf{w}\right\|_2^2$$

Despite the regularization term, the loss function remains quadratic with respect to w, allowing for closed-form optimization:

$$\hat{\mathbf{w}}_{ridge} = \left(\lambda\mathbf{I} + \mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathrm{t}$$

The term $\lambda\mathbf{I}$ is crucial in solving the singularity problem, as it transforms a non-singular matrix into a singular one with an appropriate choice of λ.

Lasso Another common regularization method is lasso, where the regularization term $L_W(\mathbf{w})$ is defined as:

$$L_W(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_1 = \frac{1}{2}\sum_{j=0}^{M-1}|w_j|$$

Thus, the overall loss function becomes:

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\left(t_i - \mathbf{w}^T\phi(x_i)\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_1$$

In this case, closed-form optimization is not possible. However, lasso typically leads to sparse regression models: when the regularization coefficient λ is large enough, some components of $\hat{\mathbf{w}}$ become equal to zero. Regularization can be seen as equivalent to minimizing $L_D(\mathbf{w})$ subject to the constraint:

$$\sum_{j=0}^{M-1}|w_j| \leq \eta$$

2.2.3 Linear regression with probability

We can approach regression in a probabilistic manner by defining a model that probabilistically maps inputs (x) to outputs (t). This model, denoted as $y(x, w)$, incorporates unknown parameters (w). We then model the likelihood, i.e., the probability that observed data $\mathcal{D}$ is generated by a given set of parameters (w), as:

$$\mathrm{P}(\mathcal{D}|\mathbf{w})$$

Finally, we estimate the parameters (w) by maximizing the likelihood:

$$\mathbf{w}_{ML} = \underset{\mathbf{w}}{\operatorname{argmax}}\,\mathrm{P}(\mathcal{D}|\mathbf{w})$$

For linear regression, we define the model as:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^T\mathbf{\Phi}(\mathbf{x}) + \epsilon$$

Here, we assume a linear model for $y(\mathbf{x}, \mathbf{w})$ and introduce noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Consequently, given a dataset $\mathcal{D}$ of N samples with inputs $\mathbf{X} = \begin{bmatrix}\mathbf{x}_1 & \dots & \mathbf{x}_n\end{bmatrix}$ and outputs $\mathbf{t} = \begin{bmatrix}t_1 & \dots & t_n\end{bmatrix}^T$, we have:

$$\mathrm{P}(\mathcal{D}|\mathbf{w}) = \mathrm{P}(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N}\mathcal{N}(t_n|\mathbf{w}^T\mathbf{\Phi}(\mathbf{x}_n), \sigma^2)$$

To find $\mathbf{w}_{ML}$, it is convenient to maximize the log-likelihood, obtaining:

$$\ell(\mathbf{w}) = \ln\mathrm{P}(t_n|\mathbf{x}_n, \mathbf{w}, \sigma^2) = -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}RSS(\mathbf{w})$$

Notice that the first part of the final formula is a constant independent of $\mathbf{w}$, so it can be ignored in maximizing the likelihood. Solving the optimization problem by setting the gradient to zero $\ell(\mathbf{w}) = 0$, yields the final formula:

$$\mathbf{w}_{ML} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{t}$$

This result aligns with the ordinary least squares approach.

This outcome allows us to interpret ordinary least squares from a probabilistic perspective, confirming that we are utilizing a normally distributed probabilistic function to generate the residuals in OLS.

Bayesian linear regression Bayesian linear regression follows a structured approach:

1. Formulation of probabilistic knowledge:
   (a) Qualitatively define the model expressing our knowledge.
   (b) Incorporate unknown parameters into the model.
   (c) Represent assumptions about these parameters with a prior distribution before observing any data.
2. Data observation.
3. Computation of posterior probability distribution for parameters:
$$\mathrm{P}(parameters|data) = \frac{\mathrm{P}(data|parameters)\mathrm{P}(parameters)}{\mathrm{P}(data)}$$
4. Utilization of Posterior Distribution to:
   - Make predictions by averaging over the posterior distribution.
   - Assess or accommodate uncertainty in parameter values.
   - Make decisions by minimizing expected posterior loss.

The posterior distribution for model parameters is derived by combining the prior with the likelihood for parameters given the data:

$$\mathrm{P}(\mathbf{w}|\mathcal{D}) = \frac{\mathrm{P}(\mathcal{D}|\mathbf{w})\mathrm{P}(\mathbf{w})}{\mathrm{P}(\mathcal{D})}$$

Here, $\mathrm{P}(\mathbf{w})$ represents the prior probability over parameters, $\mathrm{P}(\mathcal{D}|\mathbf{w})$ denotes the likelihood, and $\mathrm{P}(\mathcal{D})$ is the marginal likelihood acting as a normalization constant:

$$\mathrm{P}(\mathcal{D}) = \int \mathrm{P}(\mathcal{D}|\mathbf{w})\mathrm{P}(\mathbf{w})d\mathbf{w}$$

The mode of the posterior, known as the Maximum A Posteriori (MAP) estimate, yields the most probable value of $\mathbf{w}$ given the data.

A Gaussian likelihood assumption allows the prior to be modeled conveniently as a conjugate prior:

$$\mathrm{P}(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{S}_0)$$

Consequently, the posterior remains Gaussian:

$$\mathrm{P}(\mathbf{w}|\mathbf{t}, \mathbf{\Phi}, \sigma^2) \propto \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{S}_0)\mathcal{N}(\mathbf{t}|\mathbf{\Phi}\mathbf{w}, \sigma^2\mathbf{I})$$

Resulting in:

$$\begin{cases} \mathrm{P}(\mathbf{w}|\mathbf{t}, \mathbf{\Phi}, \sigma^2) = \mathcal{N}(\mathbf{w}|\mathbf{w}_N, \mathbf{S}_N) \\ \mathbf{w}_N = \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{w}_0 + \dfrac{\mathbf{\Phi}^T\mathbf{t}}{\sigma^2} \right) \\ \mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \dfrac{\mathbf{\Phi}^T\mathbf{\Phi}}{\sigma^2} \end{cases}$$

Prior infinitely broad When the prior distribution is infinitely broad, the Maximum A Posteriori (MAP) estimate coincides with the Maximum Likelihood (ML) solution:

$$\begin{cases} \lim_{\mathbf{S}_0 \to \infty} \mathbf{w}_N = \left(\mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{t} \\ \lim_{\mathbf{S}_0 \to \infty} \mathbf{S}_N^{-1} = \dfrac{\mathbf{\Phi}^T \mathbf{\Phi}}{\sigma^2} \end{cases}$$

This yields the ordinary least squares formula. However, in this case, we also have the covariance matrix, providing information about the related uncertainty. The only missing parameter is σ^2, which can be computed as:

$$\sigma^2 = \frac{1}{N - M} \sum_{n=1}^{N} \left(t_n - \hat{\mathbf{w}}^T (\phi)(\mathbf{x}_n)\right)^2$$

The ML estimate $\mathbf{w}_{ML}$ of $\mathbf{w}$ has the smallest variance among linear unbiased estimates and the lowest Mean Squared Error (MSE) among linear unbiased estimates (Gauss-Markov).

Prior not infinitely broad When the prior distribution is not infinitely broad, such that $\mathbf{w}_0 = 0$ and $\mathbf{S}_0 = \tau^2 \mathbf{I}$, we can express the logarithm of the posterior distribution $\mathrm{P}(\mathbf{w}|\mathbf{t})$ as:

$$\ln \mathrm{P}(\mathbf{w}|\mathbf{t}) = -\frac{1}{2\sigma^2} \sum_{i=1}^{N} \left(t_i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i)\right)^2 - \frac{1}{2\tau^2} \|\mathbf{w}\|_2^2$$

In this scenario, the Maximum A Posteriori estimate, $\mathrm{MAP}(\mathbf{w}N)$, coincides with the solution of ridge regression $\hat{\mathbf{w}}ridge$ with a regularization parameter λ set to $\lambda = \frac{\sigma^2}{\tau^2}$.

Sequential learning How to leverage the Bayesian approach for sequential learning:

1. Begin by computing the posterior with the initial data.
2. As additional data becomes available, update the prior with this new information to obtain the updated posterior.

Predictive distribution In a Bayesian framework, one can determine the probability distribution of the target variable for a new sample $\mathbf{x}^*$ (given the training data $\mathcal{D}$) by integrating over the posterior distribution:

$$\mathrm{P}(t^*|\mathbf{x}^*, \mathcal{D}) = \mathbb{E}\left[t^*|\mathbf{x}^*, \mathbf{w}, \mathcal{D}\right] = \int \mathrm{P}(t^*|\mathbf{x}^*, \mathbf{w}, \mathcal{D}) \mathrm{P}(\mathbf{w}|\mathcal{D}) d\mathbf{w}$$

This is commonly referred to as the predictive distribution. However, computing this predictive distribution typically involves the intractable task of determining the posterior distribution. Nevertheless, under certain assumptions, it is possible to compute the predictive distribution as follows:

$$\sigma_N^2(\mathbf{x}) = \sigma^2 + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})$$

Here, as the number of data points N approaches infinity, the uncertainty associated with the parameters (second term) diminishes, and the variance of the predictive distribution depends solely on the variance of the data (σ^2).

2.2.4 Challenges and limitations

Modeling presents challenges in ensuring our model effectively represents a wide range of plausible functions while maintaining informative priors without overly spreading out probabilities or assigning negligible values.

On the computational side, limitations arise with analytical integration, particularly in cases involving non-conjugate priors and complex models. Approaches like Gaussian (Laplace) approximation, Monte Carlo integration, and variational approximation become necessary for addressing these complexities and achieving accurate results.

Linear models with fixed basis functions offer several benefits:

- They permit closed-form solutions, facilitating efficient computation.
- They lend themselves to tractable Bayesian treatment, enabling principled uncertainty quantification.
- They can capture non-linear relationships by employing appropriate basis functions.

However, these models also come with several drawbacks:

- Basis functions remain static and non-adaptive to variations in the training data.
- These models are susceptible to the curse of dimensionality, particularly when dealing with high-dimensional feature spaces.

2.3 Classification

Linear classification involves learning an approximation of a function $f(x)$ that maps inputs x to discrete classes C_k (with $k = 1, \ldots, K$) from a dataset $\mathcal{D}$:

$$\mathcal{D} = \{\langle x, C_k \rangle\} \implies C_k = f(x)$$

Various approaches to classification include:

- *Discriminant function*: modeling a parametric function that directly maps inputs to classes and learning the parameters from the data.
- *Probabilistic discriminative approach*: designing a parametric model of $\mathrm{P}(C_k|\mathbf{x})$ and learning the model parameters from the data.
- *Probabilistic generative approach*: modeling $\mathrm{P}(\mathbf{x}|C_k)$ and class priors $\mathrm{P}(C_k)$, fitting models to the data, and inferring the posterior using Bayes' rule:

$$\mathrm{P}(C_k|\mathbf{x}) = \frac{\mathrm{P}(\mathbf{x}|C_k)\mathrm{P}(C_k)}{\mathrm{P}(\mathbf{x})}$$

2.3.1 Discriminant function

We begin by examining the linear discriminant functions defined as:

$$f(\mathbf{x}, \mathbf{w}) = f\left(w_0 + \sum_{j=1}^{D-1} w_j x_j\right) = f(\mathbf{x}^T\mathbf{w} + w_0)$$

Here, the function $f(\cdot)$ is not linear in $\mathbf{w}$ due to the presence of the (non-linear) activation function f, which yields either a discrete label or a probability value as its output.

The function $f(\cdot)$ partitions the input space into decision regions, with their boundaries known as decision boundaries or decision surfaces. Notably, these decision surfaces are linear functions of $\mathbf{x}$ and $\mathbf{w}$, expressed as:

$$\mathbf{x}^T\mathbf{w} + w_0 = \text{constant}$$

It's important to note that generalized linear models are more complex to utilize compared to linear models due to the incorporation of non-linear activation functions.

Labels A common encoding for two-class problems involves binary encoding, where $t \in \{0, 1\}$. In this setup, $t = 1$ indicates the positive class, while $t = 0$ denotes the negative one. Using this encoding, both t and $f(\cdot)$ represent the probability of the positive class.

Another encoding option for two-class problems is $t \in \{-1, 1\}$, which is preferable for certain algorithms.

For problems with K classes, a typical choice is the 1-of-K encoding. Here, t is a vector of length K, with a 1 in the position corresponding to the encoded class. In this encoding scheme, both t and $f(\cdot)$ represent the probability density over the classes.

Example:
For instance, in a problem with $K = 5$ classes, a data sample belonging to class 4 would be encoded as:

$$t = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \end{bmatrix}^T$$

Two-class problem The most general formulation for a discriminant linear function in a two-class linear problem is:

$$f(\mathbf{x}, \mathbf{w}) = \begin{cases} C_1 & \text{if } \mathbf{x}^T\mathbf{w} + w_0 \geq 0 \\ C_2 & \text{otherwise} \end{cases}$$

From this formulation, we can deduce the following properties:

- The decision boundary is $y(\cdot) = \mathbf{x}^T\mathbf{w} + w_0 = 0$.
- The decision boundary is orthogonal to $\mathbf{w}$.
- The distance of the decision boundary from the origin is $\frac{w_0}{\|\mathbf{w}\|_2}$.
- The distance of the decision boundary from $\mathbf{x}$ is $\frac{y(\mathbf{x})}{\|\mathbf{w}\|_2}$.

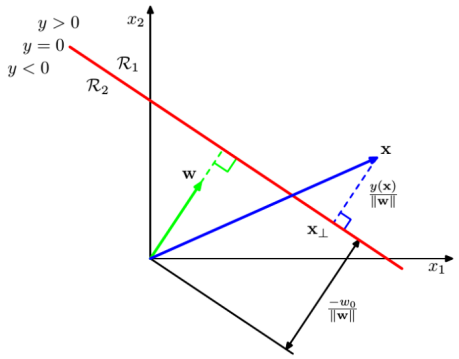


Figure 2.2: Two-class decision problem boundaries

Multiple-class problem In multiple class problems with K classes, various encoding methods can be employed:

- *One versus the rest*: this approach involves using $K-1$ binary classifiers, where each classifier distinguishes between one class (C_i) and the rest of the classes. However, this method introduces ambiguity since there may be regions mapped to multiple classes.
- *One versus one*: this method utilizes $\frac{K(K-1)}{2}$ binary classifiers, where each classifier discriminates between pairs of classes C_i and C_j. Similar to the one versus the rest approach, this method also suffers from ambiguity.

One potential solution to mitigate the ambiguity in multi-class classification is to employ K linear discriminant functions:

$$y_k(\mathbf{x}) = \mathbf{x}^T \mathbf{w}_k + w_{k0} \qquad k = 1, \ldots, K$$

In this approach, an input vector $\mathbf{x}$ is assigned to class C_k if $y_k > y_j$ for all $j \neq k$. This method ensures that the decision boundaries are singly connected and convex.

Linear basis function models Up to this point, we have focused on models operating within the input space. However, we can enhance these models by incorporating a fixed set of basis functions $\boldsymbol{\phi}(\mathbf{x})$. Essentially, this involves applying a non-linear transformation to map the input space into a feature space. Consequently, decision boundaries that are linear within the feature space would correspond to nonlinear boundaries within the input space. This extension enables the application of linear classification models to problems where samples are not linearly separable.

Ordinary least squares Let's consider a K-class problem using a 1-of-K encoding for the target. Each class is modeled with a linear function:

$$y_k(\mathbf{x}) = \mathbf{x}^T \mathbf{w}_k + w_{k0} \qquad k = 1, \ldots, K$$

In matrix notation, this can be expressed as:

$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

Here, $\tilde{\mathbf{W}}$ is of size $(D+1) \times K$, where its k-th column is denoted by $\tilde{\mathbf{w}}_k = \left(w_{k0}, \mathbf{w}_k^T\right)^T$, and $\tilde{\mathbf{x}} = \left(1, \mathbf{x}^T\right)^T$.

Given a dataset $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$ where $i = 1, \ldots, N$, we can utilize the least squares method to determine the optimal value of $\tilde{\mathbf{W}}$, resulting in:

$$\tilde{\mathbf{W}} = \left(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}\right) \tilde{\mathbf{X}}^T \tilde{\mathbf{T}}$$

Here, $\tilde{\mathbf{X}}$ is an $N \times (D+1)$ matrix with its i-th row being $\tilde{\mathbf{x}}_i^T$ and $\mathbf{T}$ is an $N \times K$ matrix with its i-th row as $\mathbf{t}_i^T$. In this setup, any new sample $\tilde{\mathbf{x}}_{new}^T$ is assigned to class C_k if $t_k > t_j$ for all j, where t_k represents the k-th component of the model output computed as $t_k = \tilde{\mathbf{x}}^T \tilde{\mathbf{w}}_k$.

The primary challenge with employing ordinary least squares in classification is that the resulting decision boundaries between regions can vary significantly based on the distribution of the data. This method may yield effective or suboptimal boundaries depending on the characteristics of the dataset.

Perceptron To address the issue of poor boundaries, one approach is to utilize a model known as the perceptron. Proposed by Rosenblatt in 1958, the perceptron is a linear discriminant model designed specifically for two-class problems, with class encoding as $\{-1, 1\}$. The perceptron model is defined as:

$$f(\mathbf{x}, \mathbf{w}) = \begin{cases} +1 & \text{if } \mathbf{x}^T\mathbf{w} + w_0 \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

The perceptron algorithm aims to determine a decision surface, also known as a separating hyperplane, by minimizing the distance of misclassified samples to the boundary. This minimization of the loss function can be achieved using stochastic gradient descent.

Although simpler loss functions could theoretically be used, they are often more complex to minimize in practice. Therefore, stochastic gradient descent is commonly employed for optimization in perceptron learning.

The core concept of the perceptron is to optimize $\mathbf{w}$ such that $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) \geq 0$ for $\mathbf{x}_i \in C_1$ and $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) < 0$ otherwise. The perceptron criterion is expressed as:

$$L_P\mathbf{w} = -\sum_{n\in\mathcal{M}} \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)t_n$$

Here, correctly classified samples do not contribute to L, and each misclassified sample $\mathbf{x}_i \in \mathcal{M}$ contributes as $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)t_n$.

Minimizing L_P is achieved using stochastic gradient descent:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha\nabla L_P(\mathbf{w}) = \mathbf{w}^{(k)} + \alpha\boldsymbol{\phi}(\mathbf{x}_n)t_n$$

Since the scale of $\mathbf{w}$ does not affect the perceptron function, the learning rate α is often set to 1. The perceptron algorithm takes a dataset $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$ where $i = 1, \ldots, N$.

Algorithm 1 Perceptron algorithm

```
Initialize w_0
k ← 0
repeat
    k ← k + 1
    n ← k mod N
    if t̂_n ≠ t_n then
        w_{k+1} ← w_k + φ(X_n)t_n
    end if
until convergence
```

Theorem 2.3.1 (Perceptron convergence)**.** *If the training dataset is linearly separable in the feature space* $\boldsymbol{\Phi}$*, then the perceptron learning algorithm is guaranteed to find an exact solution in a finite number of steps.*

Several steps may be necessary, making it challenging to distinguish between non-separable problems and slowly converging ones. If multiple solutions exist, the one obtained by the algorithm depends on the parameter initialization and the order of updates.

2.3.2 Probabilistic discriminative approaches

In a discriminative approach, we model the conditioned class probability directly:

$$\mathrm{P}(C_1|\boldsymbol{\phi}) = \frac{1}{1 + e^{-\mathbf{w}^T\boldsymbol{\phi}}} = \sigma(\mathbf{w}^T\boldsymbol{\phi})$$

Here, $\sigma(\cdot)$ denotes the sigmoidal function. This model is commonly referred to as logistic regression.

Maximum likelihood Given a dataset $\mathcal{D} = \{\mathbf{x}_i, t_i\}$, where $i = 1, \ldots, N$ and $t_i \in \{0, 1\}$, we aim to maximize the likelihood, i.e., the probability of observing the targets given the inputs $\mathrm{P}(\mathbf{t}|\mathbf{X}, \mathbf{w})$. We model the likelihood of a single sample using a Bernoulli distribution, employing the logistic regression model for conditioned class probability:

$$\mathrm{P}(t_n|\mathbf{x}_n, \mathbf{w}) = y_n^{t_n}\,(1 - y_n)^{1-t_n} \qquad y_n = \mathrm{P}(t_n = 1|\mathbf{x}_n, \mathbf{w}) = \sigma(\mathbf{w}^T\boldsymbol{\phi}_n)$$

Assuming independent sampling of data in $\mathcal{D}$, we have:

$$\mathrm{P}(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}\,(1 - y_n)^{(1-t_n)} \qquad y_n = \sigma(\mathbf{w}^T\boldsymbol{\phi}_n)$$

The negative log-likelihood (also known as cross-entropy error function) serves as a convenient loss function to minimize:

$$L(\mathbf{w}) = -\ln \mathrm{P}(\mathbf{t}|\mathbf{X}, \mathbf{w}) = -\sum_{n=1}^{N} (t_n \ln y_n + (1 - t_n)\ln(1 - y_n)) = \sum_{n=1}^{N} L_n$$

The derivative of L yields the gradient of the loss function:

$$\nabla L(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)\,\boldsymbol{\phi}_n$$

Due to the nonlinearity of the logistic regression function, a closed-form solution is not feasible. Nevertheless, the error function is convex, allowing for gradient-based optimization (even in an online learning setting).

Multi class logistic regression In multi class problems, $\mathrm{P}(C_k|\boldsymbol{\phi})$ is modeled by applying a softmax transformation to the output of K linear functions (one for each class):

$$\mathrm{P}(C_k|\boldsymbol{\phi}) = y_k(\boldsymbol{\phi}) = \frac{e^{\mathbf{w}_k^T\boldsymbol{\phi}}}{\sum_j e^{\mathbf{w}_j^T\boldsymbol{\phi}}}$$

Similar to the two-class logistic regression and assuming 1-of-K encoding for the target, we compute the likelihood as:

$$\mathrm{P}(\mathbf{T}|\boldsymbol{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{n=1}^{N} \left(\prod_{k=1}^{K} \mathrm{P}(C_k|\boldsymbol{\phi}_n)^{t_n k} \right) = \prod_{n=1}^{N} \left(\prod_{k=1}^{K} y_{nk}^{t_n k} \right)$$

As in the two-class problem, we minimize the cross-entropy error function:

$$L(\mathbf{w}_1, \ldots, \mathbf{w}_K) = -\ln \mathrm{P}(\mathbf{T}|\mathbf{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = -\sum_{n=1}^{N} \left(\sum_{k=1}^{K} t_{nk} \ln y_{nk} \right)$$

Then, we compute the gradient for each weight vector:

$$\nabla L_{\mathbf{w}_j}(\mathbf{w}_1, \ldots, \mathbf{w}_K) = \sum_{n=1}^{N} (y_{nj} - t_{nj})\, \boldsymbol{\phi}_n$$

Perceptron Replacing the logistic function with a step function in logistic regression yields the same updating rule as the perceptron algorithm.