Robot Navigation using Reinforcement Learning and Slow Feature Analysis

Diplomarbeit im Studiengang Informatik

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Eidesstattliche Erklärung

Die selbständige und eigenhändige Ausfertigung versichert an Eides statt.

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(Wendelin Böhmer)
Zusammenfassung

Bei der Anwendung von Reinforcement Learning Algorithmen auf die physische Welt muss man einen Weg finden, aus komplexen Sensordaten Umgebungszustände herauszufiltern. Obwohl die meisten bisherigen Ansätze hierfür Heuristiken verwenden, legt die Biologie nahe, dass es eine Methode geben muss, die solche Filter selbstständig konstruieren kann.

Neben der Extraktion von Umgebungszuständen müssen diese auch in einer für moderne Reinforcement Algorithmen brauchbaren Form präsentiert werden. Viele dieser Algorithmen arbeiten mit linearen Funktionen, so dass die Filter gute lineare Approximationseigenschaften aufweisen sollten.

Diese Diplomarbeit möchte eine unüberwachte Lernmethode namens Slow Feature Analysis (SFA) vorschlagen, um diese Filter zu generieren. Trainiert mit einer Zufallsfolge von Sensordaten kann SFA eine Serie von Filtern erlernen. Theoretische Betrachtungen zeigen, dass diese mit steigender Modellklasse und Trainingbeispielen zu trigonometrischen Funktionen konvergieren, welche für ihre guten linearen Approximationseigenschaften bekannt sind.

Wir haben diese Theorie mit Hilfe eines Roboters evaluiert. Als Aufgabe soll der Roboter das Navigieren in einer einfachen Umgebung erlernen, wobei der Least Squares Policy Iteration (LSPI) Algorithmus zum Einsatz kommt. Als einzigen Sensor verfügt der Roboter über eine auf seinem Kopf montierte Kamera, deren Bilder sich aber aufgrund ihrer Komplexität nicht direkt als Umgebungszustände eignen. Wir konnten zeigen, dass LSPI dank der durch SFA generierten Filter eine Erfolgsrate von ca. 80% erreichen kann.
Abstract

The application of reinforcement learning algorithms onto real life problems always bears the challenge of filtering the environmental state out of raw sensor readings. While most approaches use heuristics, biology suggests that there must exist an unsupervised method to construct such filters automatically.

Besides the extraction of environmental states, the filters have to represent them in a fashion that support modern reinforcement algorithms. Many popular algorithms use a linear architecture, so one should aim at filters that have good approximation properties in combination with linear functions.

This thesis wants to propose the unsupervised method slow feature analysis (SFA) for this task. Presented with a random sequence of sensor readings, SFA learns a set of filters. With growing model complexity and training examples, the filters converge against trigonometric polynomial functions. These are known to possess excellent approximation capabilities and should therefore support the reinforcement algorithms well.

We evaluate this claim on a robot. The task is to learn a navigational control in a simple environment using the least square policy iteration (LSPI) algorithm. The only accessible sensor is a head mounted video camera, but without meaningful filtering, video images are not suited as LSPI input. We will show that filters learned by SFA, based on a random walk video of the robot, allow the learned control to navigate successfully in ca. 80% of the test trials.
Acknowledgments

This work is based on my experience in the NeuRoBot project and on the work and help of many people. I want to thank all participants of the project.

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Mathias Franzius also deserves acknowledgment here, since his work on place cells and slow feature analysis has motivated this thesis.

At last I want to thank professor Klaus Obermayer, whose lectures and research group gave me the opportunity to enter the world of academics.

Notational conventions

Algebra notation

\[ x \quad \text{Variable } x \]
\[ \mathbf{x} \quad \text{Column vector } x \]
\[ [x_1, \ldots, x_n] \quad \text{An } n \text{ dimensional row vector with entries } x_i \]
\[ \mathbf{0} \quad \text{A vector with all entries being } 0 \]
\[ \mathbf{1} \quad \text{A vector with all entries being } 1 \]
\[ \mathbf{M} \quad \text{Matrix } \mathbf{M} \]
\[ \mathbf{I} \quad \text{The identity matrix} \]
\[ \mathbf{M}^\top \quad \text{The transpose of matrix } \mathbf{M} \in \mathbb{R}^{n \times m} : \forall ij : M^\top_{ij} = M_{ji} \]
\[ \text{tr}(\mathbf{M}) \quad \text{The trace of matrix } \mathbf{M} \in \mathbb{R}^{n \times n} : \text{tr}(\mathbf{M}) = \sum_{i=1}^{n} M_{ii} \]
\[ ||\mathbf{x}|| \quad \text{Arbitrary norm of vector } \mathbf{x} \]
\[ ||\mathbf{x}||_2 \quad \text{L}_2\text{-norm of vector } \mathbf{x} \in \mathbb{R}^n : ||\mathbf{x}||_2 = \sqrt{\sum_{i=1}^{n} x_i^2} \]
\[ ||\mathbf{M}||_F \quad \text{Frobenius norm of matrix } \mathbf{M} \in \mathbb{R}^{n \times m} : \]
\[ ||\mathbf{M}||_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{m} M_{ij}^2} = \sqrt{\text{tr}(\mathbf{M}^\top \mathbf{M})} = \sqrt{\text{tr}(\mathbf{M} \mathbf{M}^\top)} \]
Analysis notation

- $\mathcal{A}$: Set $A$
- $\emptyset$: The empty set
- $[a, b]$: The real interval between $a$ and $b$: $[a, b] = \{x | a \leq x \leq b\} \subset \mathbb{R}$
- $\mathcal{A} \times \mathcal{B}$: The set of all tuples $(a, b)$ with $a \in \mathcal{A}$ and $b \in \mathcal{B}$
- $|\mathcal{A}|$: The cardinality of set $\mathcal{A}$
- $\mathcal{P}(\mathcal{A})$: The power set of set $\mathcal{A}$
- $f(x)$: Function $f : \mathcal{A} \to \mathcal{B}$
- $\nabla f(x)_{|x_0}$: The gradient of function $f : \mathcal{A} \to \mathcal{B}$ with respect to its argument $x \in \mathcal{A}$ at position $x_0$: $\nabla f(x)_{|x_0} = \frac{\partial f(x)}{\partial x}|_{x_0}$

Statistics notation

- $\mathbb{E}[x]$ : The expectation of the random variable $x$ with distribution function $p(x)$: $\mathbb{E}[x] = \int x \ p(x) \ dx$
- $\mathbb{E}_t[f(t)]$: The expectation over all $n$ realizations of variable $t$, normally the empirical mean over index $t$: $\mathbb{E}_t[f(t)] = \frac{1}{n} \sum_{t=1}^{n} f(t)$
- $\mathbb{C}[x, y]$: The covariance between random variables $x$ and $y$ with joint distribution function $p(x, y)$:
- $\mathbb{C}[x, y] = \text{cov}(x, y) = \int \int (x - \mathbb{E}[x]) \ (y - \mathbb{E}[y]) \ p(x, y) \ dx \ dy$
- $\mathbb{C}[x]$: The covariance matrix of the random vector $x$, i.e. the covariance between all entries: $(\mathbb{C}[x])_{ij} = \mathbb{C}[x_i, x_j]$
- $\mathbb{V}[x]$: The variance of the random variable $x$: $\mathbb{V}[x] = \mathbb{C}[x, x]$
- $x \sim p(y, \cdot)$ : The random variable $x \in \mathcal{X}$ is drawn according to the distribution function $p : \mathcal{Y} \times \mathcal{X} \to [0, 1]$, where $\forall y \in \mathcal{Y} : \sum_{x \in \mathcal{X}} p(y, x) = 1$
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Chapter 1

Introduction

Modern robotics faces a major drawback.

Over the last decades, hard- and software has matured into commercially applicable products. Nowadays, robotic control is able to cross deserts, navigate independently on other planets and even climb stairs on two legs. That is, if the robot is fine tuned to the course, operators stand by to correct inevitable jams and stairs have the right height and form. Modern robotic control is not very adaptive.

The scientific discipline of adaptive control, on the other hand, is developed and tested mainly on discrete, small sized toy examples. Complex sensory input, uncertain and noise afflicted, is not compatible with these standard methods. A natural way to merge these two technologies is to find a preprocessing - a process that strips the essential information from raw sensor data.

But what is essential information? Surely we can only answer this question in context of the individual control domain at hand. But whatever choice we make, we can be certain that we will forget something. An ideal preprocessing would also adapt to the control domain on its own.

In this thesis we want to investigate the properties of an unsupervised technique, called slow feature analysis, as an auto-adaptive preprocessing in the domain of environment specific navigational control.

1.1 Motivation

Roughly 35 years ago, biologists discovered a cluster of cells in the hippocampal area of rodents, which encode the spatial position of the animal. Within minutes of seemingly random movement in an unknown environment, the cells specialize to fire only around one position each. Moreover, the cell population covers the whole accessible area, which lead many scientists to believe that the so called place cells are a preliminary stage of the rodents navigational control [44].

How these cells adapt, on the other hand, is still a question open to debate. Until recently, the only explanation was the so called path integration, a tech-
nique in which the rodent integrates its movement up to estimate the current position. Since the sense of movement can be flawed, small mistakes will sum up over time and have to be corrected by external stimuli, which have to be identified in the environment, first. The computational approach to this problem, used in robotics, is called simultaneous localization and mapping (SLAM) and will be discussed as an alternative to our approach in section 5.1.7.

Last year, Franzius et al. [42] were able to show that a memoryless feed forward network is able to learn place cell behaviour. The network adapts to videos of a head mounted camera (substitutional for the rodent's eyes) by an unsupervised learning technique called slow feature analysis (SFA).

Reinforcement learning (or neuro-dynamic programming) is a method to learn a control based on reward and punishment. A set of rewarded/punished example movements is generalized to estimate the expected sum of future rewards (value) at every position and for every possible action. Given a current position, the so called state of the system, the control chooses the action that promises the highest value. Obviously, the efficiency of this approach depends on how well the value can be estimated, which in return depends on the coding of the state.

Place cells provide an intuitive coding for linear architectures. Weighting every cells output with the mean value of its active region can summed up approximate any value function up to a quality depending on the number of cells. Therefore, the place cells of Franzius et al. should be a natural (and biological plausible) preprocessing for linear value estimators.

As it turns out, properly trained SFA produces a mapping of video images into corresponding trigonometric polynomials in the space of robot positions. Franzius' place cells were products of an additional step independent component analysis (ICA) which does not influence the linear approximation quality and can therefore be omitted.

The goal of this thesis is to formulate this basic idea into a working procedure and to demonstrate its soundness in a real world robot navigation experiment.

1.2 Method

We want to learn a preprocessing using slow feature analysis (SFA) out of the video images of a robots head mounted camera. This preprocessing should represent the robots position and orientation (its state) in a fashion suitable for linear function approximation. With this state at hand, we want to use the reinforcement learning method policy iteration (PI) to learn a control for the robot.

Note that the preprocessing is adapted to one environment, e.g. one room only, and will not work anywhere else. However, the same is true for any control learned by reinforcement learning, so SFA fits well within this framework.

Both SFA and PI need an initial random walk, crossing the whole environment. Therefore the robot has to drive around by choosing random actions,
1.2. METHOD

First. The only needed sensor information of this phase is the video of a head mounted camera. However, for the reinforcement method, we also need to record the reward and punishment at every step. As simple task, the robot receives reward for entering a goal area and punishment for getting too close to walls. The resulting control should drive into the goal area as quickly as possible, while keeping its distance to walls.

Secondly, SFA will learn a series of filters based on the recorded video. The output of these filters, applied on the initial video, is used as input of policy iteration. PI estimates the expected sum of future rewards (value) for every action and position.

Control With the value estimator at hand, or to be precise its parameter vectors \(w^{(1)}, \ldots, w^{(a)}\) (one for every action), the control works as depicted in figure 1.1:

(a) The robot starts in an unknown position and wishes to navigate into a goal area, marked with a G for demonstration purposes.

(b) A head mounted video camera shoots a picture \(I(x, y, \theta)\) out of the current perspective.

(c) The series of filters \(\phi_1 \ldots \phi_n\), learned by slow feature analysis, produce one real valued output \(\phi_i(x, y, \theta)\), each. For every possible action, the output is multiplied by a weight vector \(w_i\), found by reinforcement learning. The sum of the weighted outputs is the value estimation \(V^a(x, y, \theta)\) of this action.

(d) The robot executes the action with the highest value and repeats the procedure until it reaches the goal.

Figure 1.1: Proposed methodology. See text for a description.
**CHAPTER 1. INTRODUCTION**

**Multiple tasks** The reinforcement method employed in this thesis, *least squares policy iteration* (LSPI), chooses the most promising in a finite number of actions \(a\), based on the current state \(x \in \mathbb{R}^d\). Unfortunately, its complexity is \(O(d^3 a^3)\) in time and \(O(d^2 a^2)\) in space. An efficient kernel SFA algorithm itself has a complexity of at least \(O(m^3)\) in time and \(O(m^2)\) in space, where \(m\) is the number of support vectors (comparable to \(d\)). So why not use a kernel version of LSPI when there is no significant advantage to the proposed method in computational complexity?

For once, LSPIs complexity also depends on the number of actions \(a\). An SFA preprocessing can use the available memory up to \(O(m^2)\) to produce a number of filters \(d \ll m\). This way one can consider a much larger number of actions. More importantly, the state space extracted by SFA can be used in more than one reinforcement problem. For example, when the robot should learn two tasks, one can learn both given the same initial video but different rewards. Therefore, determining the preprocessing once allows to learn multiple tasks quickly afterwards.

**Theory** In chapter 3 the theoretical background of reinforcement learning is presented as well as the complete derivation of LSPI with all necessary algorithms.

Chapter 4 describes slow feature analysis theoretically. It also contains an overview of recent applications and algorithms, including a novel derivation of a kernelized algorithm.

Both chapters are based on common concepts of machine learning and kernel techniques, which are introduced for the sake of completeness in chapter 2.

### 1.3 Experiments

Within the NeuRoBot project, the author was able to perform experiments with a real robot. To check the theoretical predictions, we constructed a rectangular area with tilted tables, in which the robot should navigate towards some virtual goal area. We tested two goal areas, which were not marked or discriminable otherwise besides the reward given in training.

To evaluate the proposed method less time consuming, the author also implemented a simulated version of the above experiment. At last, theoretical predictions exist only for rectangular environments. To test the behaviour outside this limitation, we used the simulator to create an environment consisting of two connected rooms.

A detailed description of these experiments, as well as a thorough analysis of both SFA and LSPI under optimal conditions, can be found in chapter 5. The authors conclusions and an outlook of possible future works are presented in chapter 6.
Chapter 2

Preliminaries

In this chapter we introduce the reader to the general concepts of machine learning, especially to linear models (at the example of least squares regression) in section 2.1 and kernel techniques (with some less common procedures we will need in this thesis) in section 2.2.

We will start with a general introduction of regression (sec. 2.1 and 2.1.1), followed by a discussion of convexity (sec. 2.1.2), model choices (sec. 2.1.3) and validation techniques (sec. 2.1.4). On this basis, we will finally define two commonly used linear regression algorithms: least squares regression and ridge regression (sec. 2.1.5).

In the second part, we will give an overview on kernel techniques (sec. 2.2 and 2.2.1), demonstrate them on a kernel regression algorithm (sec. 2.2.2), discuss a kernelized version of the covariance eigenvalue problem (sec. 2.2.4) and end with kernel matrix approximation methods (sec. 2.2.5) and a corresponding support vector selection algorithm (sec. 2.2.6).

2.1 Regression

We live in a world where things follow causal relationships, which should be expressible as functions of observations (i.e. products of the real "causes"). The exact nature and design of these relationships are unknown but might be inferred from past observations. To complicate things even further, these observations can also be afflicted by noise, i.e. random distortions independent of the real "cause". Regression deals with inference of functional relationships from past observations, based on some simplifying assumptions.

Assumption 2.1 The random variable $t \in \mathcal{T}$ depends on the observation $x \in \mathcal{X}$ by $t = f(x) + \eta$ with $\eta \in \mathcal{T}$ being another zero mean random variable.

We assume that some kind of observation yields an input sample $x$, which can be assigned a target value by $t$ by an expert or process of nature. Due to errors in this process, $t$ is distorted by a random variable $\eta$, independent of $x$. 
Estimating the volume inside a balloon based on its diameter would be an example. Clearly there is a relationship, but since real balloons do not follow ideal mathematical shapes, it is hard to find. Physicists would take measurements of balloon diameters (the input samples) and air volumes (the target values) to find a function which explains most measurements with a minimum amount of noise. Since measurements are prone to be inexact and the rubber of individual balloons differs slightly, we have to expect some noise in the target values. An exact reproduction of the observed target values will therefore reproduce measure errors and mispredict unseen future inputs. The physicists approach to this problem is formulated as Ockhams razor, which in short states that theories have to be simple as well as explanatory.

In the following, we will denote $S = \{(x^{(1)}, t^{(1)}), \ldots, (x^{(n)}, t^{(n)})\} \in \mathcal{P}(X \times \mathcal{Y})$ as the training set. Regression aims to estimate the function $f(x)$ based only on this data. The balance of Ockhams razor is difficult to maintain and led to a variety of regression algorithms.

### 2.1.1 Optimization problem

We wish to find a function $y : X \rightarrow \mathcal{Y}$ which estimates the real (but unknown) relationship $f$. The only knowledge available is the training set $S$, so we construct a cost function $C$ which defines the optimization goal indirectly by comparing the target values with the predictions made by some given function $y$.

**Definition 2.2 (Cost function)**

A cost function has the form $C : (X \rightarrow \mathcal{Y}) \times \mathcal{P}(X \times \mathcal{Y}) \rightarrow \mathbb{R}$.

The intuition is that the cost function is small if $f$ is applied, and hopefully also small for functions similar to $f$. Minimizing $C$ with respect to $y$ should therefore lead to a similar function.

The approach suggesting itself is to evaluate $y$ at every sample $x^{(i)}$ and consider the distance under some norm $\| \cdot \|$ to target $t^{(i)}$ as the empirical cost for this sample. Because we have no reason to favor any sample, we sum up the individual costs and the result is called the empirical cost function $C_{\text{emp}}$:

$$ C_{\text{emp}}(y, S) = \sum_{j=1}^{n} \| y(x^{(j)}) - t^{(j)} \| $$

(2.1)

Note that, due to the norm, the noise term $\eta$ in assumption 2.1 will not cancel out. The only way for $C$ to reach zero is to reproduce the noise of $t$ in $y$, which is not desirable.

If we wish to avoid this problem, we can invoke Ockhams razor and penalize complex functions with a regularization term $R(y) \in \mathbb{R}$. A less complex function will be less likely to reproduce the observed noise and therefore predict unseen data better. Examples for $R$ would be the length of the parameter vector (linear functions), the number of support vectors (kernel machines) or the number of
hidden neurons (neuronal networks). Together with the empirical cost we obtain
the regularized cost function \[ C_{reg}(y, S) = \sum_{j=1}^{n} ||y(x^{(j)}) - t^{(j)}|| + R(y) \] (2.2)
Note that the regularization term \( R(y) \) is independent of the sample size \( n \) and
with growing \( n \) will lose relevance. Section 2.1.4 will discuss the effects of
sample size in more detail.

**Definition 2.3 (Optimal function)** The global minimum of a cost function
\( C(y, S) \) with respect to \( y \) is called optimal function \( y^* \) of \( C \):
\[
y^* = \arg \min_y C(y, S) \quad (2.3)
\]
The optimal function \( y^* \) of \( C \) is the function we were looking for and should
resemble \( f \) at least on the training set. Arbitrary functions can not be repre-
sented in a computer, so a common approach chooses a parameterized function
class \( \mathcal{F} \subset (\mathbb{X} \rightarrow \mathbb{Y}) \) to pick \( y = \mathcal{F}(w) \) from.

One approach to find the optimal function is to calculate the gradient of \( C \)
with respect to the function class parameters \( w \) at an arbitrary start position
\( w_0 \). One can follow the negative gradient \( -\nabla C|_{w_0} \) in small steps, leading to
smaller costs if the step size is well chosen. This method is called gradient
descent [1].

The disadvantage is that the method will stop at every \( w \) that fulfills \( \nabla C|_{w} = 0 \), called an extremum of \( C \). Depending on the considered function class \( \mathcal{F} \)
the cost function can have multiple extrema with respect to the parameters \( w \), and
not all have to be global minima after definition 2.3. In other words, gradient
descent will converge to whatever extrema the gradient lead to, starting at \( w_0 \).
This means we can never be sure that we reached a global minimum, if no closed
solution of \( \nabla C \) is possible.

Keeping this in mind, it is wise to choose \( \mathcal{F} \) such that every extrema of the
cost function is a global minimum, ideally the only one. In this thesis we will
focus on convex functions.

#### 2.1.2 Convexity

There are other functions without local minima, but convex functions provide
other desirable mathematic properties (see [7] for details). In some special cases
it is even possible to derive a closed analytical solution (section 2.1.4).

**Definition 2.4 (Convex function [7])** A function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) is convex if
dom \( f \) is a convex set and if for all \( x, y \in \text{dom} f \), and \( \theta \) with \( 0 \leq \theta \leq 1 \), we have
\[
f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y). \quad (2.4)
\]

\[^1\] If also \( \nabla C|_{w} > 0 \) we speak of a minimum, but not necessarily a global minimum.
We can tighten the definition further. When the strict inequality in equation 2.4 holds, we speak of a \textit{strictly convex function}. These have the additional advantage that the minimum is \textit{unique}, i.e. no other extrema exists.

Anyway, the main property we are interested in both cases is that every extrema is a global minimum:

\textbf{Proposition 2.1 (First order convexity condition \cite{7})} Suppose $f$ is differentiable (i.e. its gradient $\nabla f$ exists at each point in $\text{dom } f$, which is open). Then $f$ is convex if and only if $\text{dom } f$ is convex and

$$f(y) \geq f(x) + \nabla f(x)^\top(y - x) \tag{2.5}$$

holds for all $x, y \in \text{dom } f$.

\textbf{Proof:} See \cite{7}.

Every extrema $x$ of $f$ satisfies $\nabla f(x) = 0$. According to proposition 2.1, if $f$ is convex then $\forall y \in \text{dom } f : f(y) \geq f(x)$, which identifies $x$ as a global minimum of $f$.

However, we do not necessarily wish the functions $y \in F$ but the discussed cost functions to be convex:

\textbf{Proposition 2.2 (Convex cost function)} Let $S \in \mathcal{P}(X \times T)$ be arbitrary but given. If $R(y)$ and all $y \in F$ are convex functions then the cost functions (eq. 2.1) and (eq. 2.2) are convex in the domain $F$.

\textbf{Proof:} $y(x^{(j)})$ and $-t^{(j)}$ are convex, and how lemma 2.3 shows, the sum of them is convex too. Lemma 2.4 proves that norms are convex, so their sum has to be, too. At last, $C^\text{emp}$ and $R(y)$ are convex, and so is their sum $C^\text{reg}$. \hfill $\square$

\textbf{Lemma 2.3 (Pointwise sum \cite{7})} The pointwise sum of two convex functions $f_1$ and $f_2$, $f = f_1 + f_2$ with $\text{dom } f = \text{dom } f_1 \cap \text{dom } f_2$, is a convex function.

\textbf{Proof:} Insert $(\theta x + (1 - \theta)y)$ into $f_1(\cdot) + f_2(\cdot)$ and apply (eq. 2.4) two times. \hfill $\square$

\textbf{Lemma 2.4 (Norms \cite{7})} Every norm on $\mathbb{R}^n$ is convex.

\textbf{Proof:} If $f : \mathbb{R}^n \to \mathbb{R}$ is a norm, and $0 \leq \theta \leq 1$, then

$$f(\theta x + (1 - \theta)y) \leq f(\theta x) + f((1 - \theta)y) = \theta f(x) + (1 - \theta)f(y).$$

The inequality follows from the triangle inequality, and the equality follows from homogeneity of a norm. \hfill $\square$

\subsection{Function classes}

Convexity of the cost function depends on its formulation and the considered function class $F \subset (X \to T)$. The family of convex functions is large (see \cite{7} for examples). However, we want to introduce two classes that will play a mayor role in this thesis because they allow a closed analytical solution under the squared $L_2$ norm.
2.1. REGRESSION

Definition 2.5 (Linear function \[7\]) A function \( f : \mathbb{R}^p \rightarrow \mathbb{R}^q \) is linear if for all \( x, y \in \mathbb{R}^p \) and \( \alpha, \beta \in \mathbb{R} \) it satisfies the condition
\[
f(\alpha x + \beta y) = \alpha f(x) + \beta f(y).
\] (2.6)

Linear functions have nice analytical properties, e.g. they can be uniquely determined by a matrix \( W \in \mathbb{R}^{p \times q} \): \( f(x) = W^\top x \). Convexity be seen by comparison of (eq. 2.6) and (eq. 2.4).

Definition 2.6 (Affine function \[7\]) An affine function \( f : \mathbb{R}^p \rightarrow \mathbb{R}^q \) is the sum of a linear function and a constant: \( f(x) = W^\top x + b \).

The bias \( b \) violates the linear condition, but affine functions share many properties with linear functions. They can express more relationships, however. For example, a line that does not cross the origin can be expressed as an affine, but not as a linear function.

By extending the input vector \( x \) by a constant (i.e. \( x_0 = 1 \)) one can express an affine function as a linear function. This trick can be applied if the algorithm at hand requires linearity but the data can only be properly predicted by an affine function.

Lemma 2.5 Affine functions are convex.

Proof: We show convexity for every component \( f_i(x) = w_i^\top x + b_i \).
\[
f_i(\theta x + (1 - \theta)y) = w_i^\top (\theta x + (1 - \theta)y) + b_i
\]
\[
= \theta w_i^\top x + (1 - \theta) w_i^\top y + (1 - \theta + \theta) b_i
\]
\[
= \theta f_i(x) + (1 - \theta) f_i(y)
\]

\[\square\]

2.1.4 Validation

In regression, we do not know the real target function \( f \) of assumption 2.1, but aim to find a "similar" function \( y \in F \). Since we can not construct a similarity measure between \( f \) and \( y \) directly, we define a cost function instead. Though one can obtain an \( y^* \) optimal to the cost function, the approach is susceptible to many sources of error:

- The cost function can be chosen differently, leading to different optimal functions. Here the choice of regularized vs. empirical arises as well as the choice of the regularization term. Anyway, the two presented equations are not the only imaginable cost functions (see \[1\] for more).
- The considered function class \( F \) might not be suited for the data at hand. On the one hand, \( F \) can be too weak, e.g. a parabola can not be represented by a linear function. If, on the other hand, the sample size \( n \) is too small, \( y^* \) can reduce the individual costs of all training samples to zero, but take unreasonable values between them. This effect is called over-fitting \[9\].
The training sets sampling might introduce errors. If a region of \( X \) is left out, \( f \) can not be estimated there. More general, unbalanced sampling leads to a good estimation of \( f \) where many samples are available, but a poor estimation where this is not the case. The sum of the individual costs tolerates big errors in rarely sampled regions, if it means to shrink the error in highly sampled regions even slightly. This effect is also influenced by the choice of \( F \). Especially linear and affine functions are known to react badly to unbalanced sampling [9].

The last point can be circumnavigated if one can ensure identical and independent distributed (iid) sampling. This way, given enough samples, the training set will be sampled homogeneously from \( X \). However, in most practical cases one can not give such a guaranty.

The common procedure to validate \( y^* \) is to withhold a test set \( S' \subseteq \mathcal{P}(X \times T) \), \( S' \cap S = \emptyset \) from the training. A comparison of the normalized empirical costs of training and test set (called training and test error) demonstrates how well \( y^* \) generalizes. If the errors are approximately the same, the optimal function predicts unseen inputs obviously as well as the training samples. However, if the test error is significantly higher than the training error, \( y^* \) is probably overfitting. Counter measures would include more training samples, a less complex function class or stronger regularization.

Another useful test is the computation of \( y^* \) for the same cost function and training data, but a different function class \( F \). The comparison of the test and training errors can tell us which function class is better suited. Especially if one can choose the complexity in a family of function classes (e.g. number of support vectors in kernel machines), it is interesting at which complexity the error saturates. Finding this point (i.e. the simplest model which estimates \( f \) well) is sometimes referred to as model selection or model comparison [9].

**Algorithm 1** Linear Least Squares Regression

| Require: \( x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^p; t^{(1)}, \ldots, t^{(n)} \in \mathbb{R}^q \) |
| \( C_0 = \text{zeros}(p,p) \) |
| \( B_0 = \text{zeros}(p,q) \) |
| for \( i = 1, \ldots, n \) do |
| \( C_i = C_{i-1} + x^{(i)}x^{(i)\top} \) |
| \( B_i = B_{i-1} + x^{(i)}t^{(i)\top} \) |
| end for |
| \( W = \text{inv}(C_n)B_n \) |
| return \( W \) |
2.1.5 Linear regression algorithms

The least squares regression problem applies the squared $L_2$ norm and the class of linear functions on the empirical cost function (eq 2.1):

$$C_{\text{emp}}(y,S) = \sum_{j=1}^{n} \| y(x^{(j)}) - t^{(j)} \|_2^2 = \| W^\top X - T \|_F^2$$

where $\| \cdot \|_F^2$ is the squared Frobenius norm and the matrices $X_{ij} = x_i^{(j)}$ and $T_{ij} = t_i^{(j)}$ are introduced for simplicity.

Extending the input samples by a constant (i.e. $x_0 = 1$) allows us to use the same formulation for the class of affine functions.

To find the optimal function $y^*(x) = W^\top x$ we set the derivation of equation 2.7 with respect to the parameter matrix $W$ to zero:

$$\frac{\partial C_{\text{emp}}(W,S)}{\partial W} = 2XX^\top W - 2XT^\top \overset{!}{=} 0$$

$$\Rightarrow W^* = (XX^\top)^{-1}XT^\top$$

which holds, providing the rows of $X$ are linearly independent and the covariance matrix $XX^\top$ therefore of full rank.

We can also use the regularized cost function (eq. 2.2) with the regularization term $R(y) = R(W) = \lambda \text{tr}(W^\top W)$ which penalizes the squared $L_2$ norm of the column vectors of $W$. $\lambda \in \mathbb{R}$ regulates how strong the penalty for complex functions is.

$$\frac{\partial C_{\text{reg}}(W,S)}{\partial W} = 2XX^\top W - 2XT^\top + 2\lambda W \overset{!}{=} 0$$

$$\Rightarrow W^* = (XX^\top + \lambda I)^{-1}XT^\top$$

Regression with this regularization term is known as ridge regression [9] or in the context of neural networks as weight decay [1].

Both algorithms have a complexity of $O(p^2)$ in space and max($O(np^2), O(p^3)$) in time. The $O(p^3)$ term originates in the matrix inversion.

**Algorithm 2 Linear Ridge Regression**

**Require:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^p; t^{(1)}, \ldots, t^{(n)} \in \mathbb{R}^q; \lambda \in \mathbb{R}$

C\_0 = zeros(p,p)
B\_0 = zeros(p,q)
for $i = 1, \ldots, n$ do
C\_i = C\_i-1 + x^{(i)} x^{(i)}\top
B\_i = B\_i-1 + x^{(i)} t^{(i)}\top
end for
W = inv(C\_n + \lambda I)B\_n
return W
CHAPTER 2. PRELIMINARIES

2.2 Kernel techniques

Realistic processes can seldom be approximated sufficiently with linear function classes. Classes of nonlinear functions (e.g. neural networks) could provide satisfactory results, but their cost functions are rarely convex and the optimization therefore complicated.

Another approach is the nonlinear expansion of the input samples \( x \in \mathcal{X} \). This way, projected into a high dimensional feature space, the problem can be treated as linear, while the solution in original space \( \mathcal{X} \) is nonlinear. The classic example to demonstrate this is the XOR problem.

In the XOR problem, the input \( x \in \{0, 1\}^2 \) and the target \( t \in \{0, 1\} \) are connected by a simple rule: If both entries of \( x \) are the same then \( t = 0 \), otherwise \( t = 1 \). It is easy to see that there is no linear function \( y(x) = w^\top x \) that solves this problem, but if we expand the input vector \( x' = [x_1, x_2, x_1x_2]^\top \), the parameter vector \( w = [1, 1, -2]^\top \) explains the relationship perfectly. Thus, with the suggested expansion, the XOR problem is linearly solvable.

Expansion almost always increases the dimensionality of the input. The fact that one normally does not know the perfect expansion beforehand rarely lead to feasible expansions that solve the problem. In the case that a suitable expansion size would outnumber the number of training samples, the kernel trick can be employed.

2.2.1 The kernel trick

The kernel trick defines the nonlinear expansion indirectly. One exploits the representer theorem, which states that the optimal function of a cost function can be represented as scalar products of the training set.

Kernels are a broad class of functions, which are equivalent to a scalar product in a corresponding vector space. The intuition of the kernel trick is to exchange the euclidian scalar product by one in a high dimensional nonlinear feature space, i.e. another kernel.

Choosing a nonlinear kernel is equivalent to a nonlinear expansion of the input vector. This way one can handle huge feature spaces. The drawback is that the optimal function depends on scalar products to all training samples, which can be infeasible for large sample sizes.

In the following we introduce the elements of kernel methods used in this thesis. To follow the derivation path in full length, the reader is referred to [4].

Definition 2.7 ((Positive definite) kernel [4]) Let \( \mathcal{X} \) be an nonempty set. A function \( k \) on \( \mathcal{X} \times \mathcal{X} \) which for all \( n \in \mathbb{N} \) and all \( x^{(1)}, \ldots, x^{(n)} \in \mathcal{X} \) gives rise to a positive definite Gram matrix is called a positive definite kernel.

For a definition of Gram matrix and positive definite matrix, see [4].

One can prove that every positive definite kernel function uniquely implies a scalar product \( \langle \psi(x), \psi(x') \rangle = k(x, x') \) with \( \psi(x) \) being the projection of \( x \in \mathcal{X} \) into another space.
2.2. KERNEL TECHNIQUES

To be more exact, one can show that a kernel function implies a reproducing kernel Hilbert space (RKHS) of functions \( f : \mathcal{X} \to \mathbb{R} \) with a scalar product. With a detour over Mercer kernels (which are equivalent to positive definite kernels) one can show that it is possible to construct a mapping \( \psi(\cdot) \) for which \( k(\cdot, \cdot) \) acts as a dot product.

In the following we will refer to an arbitrary kernel function \( k(\cdot, \cdot) = \langle \psi(\cdot), \psi(\cdot) \rangle_\mathcal{H} \) in the corresponding RKHS \( \mathcal{H} \).

**Theorem 2.6 (Representer Theorem [4])** Denote by \( R : [0, \infty) \to \mathbb{R} \) a strictly monotonic increasing function, by \( \mathcal{X} \) a set and by \( C : (\mathcal{X}, \mathbb{R}, \mathbb{R})^n \to \mathbb{R} \cup \{\infty\} \) an arbitrary loss function. Then each minimizer \( y : \mathcal{X} \to \mathbb{R} \) of the regularized risk

\[
C((x^{(1)}, t^{(1)}, y(x^{(1)})), \ldots, (x^{(n)}, t^{(n)}, y(x^{(n)}))) + R(||y||_\mathcal{H}) \quad (2.9)
\]

admits a representation of the form

\[
y(x) = \sum_{i=1}^{n} \alpha_i k(x^{(i)}, x). \quad (2.10)
\]

**Proof:** See [4]. Note that a loss function is a slightly different defined cost function and regularized risk a cost function with a regularization term.

Multivariate functions \( y : \mathbb{R}^p \to \mathbb{R}^q \) can be represented component wise \( y_j(x) = \sum_{i=1}^{n} A_{ij} k(x^{(i)}, x) \), giving rise to a new parameter matrix \( A \in \mathbb{R}^{n \times q} 
\]

\[
y(x) = A^\top k(x) \quad (2.11)
\]

where \( k(x) = [k(x^{(1)}, x), \ldots, k(x^{(n)}, x)]^\top \) is called a kernel expansion of \( x \).

**Remark 2.1 ("Kernel trick" [4])** Given an algorithm which is formulated in terms of a positive definite kernel \( k \), one can construct an alternative algorithm by replacing \( k \) by another positive definite kernel.

The kernel trick allows the replacement of scalar products (which are positive definite kernels) by complex, nonlinear kernels. One can take this replacement as a projection \( \psi(\cdot) \) into a high dimensional feature space. In this space, we can solve our optimization problem linear. The only restriction is that the original algorithm must be formulated entirely with scalar products.
Algorithm 3 Kernelized Ridge Regression

Require: \( x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^p; t^{(1)}, \ldots, t^{(n)} \in \mathbb{R}^q; \lambda \in \mathbb{R}; k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R} \)

\[
K = \text{zeros}(n,n) \\
\text{for } i = 1, \ldots, n \text{ do} \\
\quad \text{for } j = 1, \ldots, n \text{ do} \\
\quad \quad K_{ij} = k(x^{(i)}, x^{(j)}) \\
\quad \text{end for} \\
\text{end for} \\
A = \text{inv}(K + \lambda I)^T \\
\]

2.2.2 Kernelized regression

To demonstrate the kernel trick, we will derive a kernelized version of the linear ridge regression algorithm.

First we have to notice that there are no scalar products in algorithm 2. Therefore, it is necessary to reformulate the algorithm \[9\]. Again, we start by setting the derivation of \( C_{reg} \) with respect to \( W \) to zero:

\[
\frac{\partial C_{reg}(W, S)}{\partial W} = 2X^T W - 2XT^T + 2\lambda W \overset{!}{=} 0 \\
\Rightarrow W^* = -\frac{1}{\lambda}(XX^T W - XT^T) = XA
\]  \hspace{1cm} (2.12)

with \( A = -\frac{1}{\lambda}(X^T W^* - T^T) \). Next we will clear \( A \) of its dependency on \( W^* \). Substituting (eq. 2.12) in \( C_{reg} \) and the derivation with respect to \( A \) yields:

\[
C_{reg}(A, S) = \text{tr}((A^T X^T X - T)^2) = \text{tr}((A^T K - T)^2) \\
\frac{\partial C_{reg}(A, S)}{\partial A} = 2KK^T A - 2KT^T + 2\lambda KA \overset{!}{=} 0 \\
\Rightarrow A^* = (K + \lambda I)^{-1}T^T
\]

where the Gram matrix of scalar products \( K_{ij} = x^{(i)^T} x^{(j)} \in \mathbb{R}^{n \times n} \) can be replaced by any other kernel matrix \( K'_{ij} = k(x^{(i)}, x^{(j)}) \). Prediction follows (eq. 2.11):

\[
y(x) = W^T x = A^{*T}X^T x = A^{*T}k(x)
\]  \hspace{1cm} (2.13)

The complexity of this algorithm is \( O(n^2) \) in space and \( O(n^3) \) in time.
2.2. KERNEL TECHNIQUES

2.2.3 Kernels

Since the kernel implies the feature space, choosing a nonlinear expansion is equivalent to choosing a kernel. Therefore it is necessary to know common kernel functions and their properties.

**Polynomial kernels** As we have seen in the XOR example, a polynomial expansion can be useful. The direct approach would be to collect all multivariate monomials up to degree \( d \) in a vector. For \( p \) dimensional input vectors, the expanded vector would have dimensionality \( (d+p-1)! \). The corresponding kernel function

\[
k(x, x') = (x^\top x' + 1)^d
\]

(2.14) projects into the same space of polynomials with degree \( \leq d \). To demonstrate this let us consider the following example [9]: The input vectors shall be \( x, x' \in \mathbb{R}^2 \). The polynomial kernel function of degree 2 for those two is:

\[
k(x, x') = (x^\top x' + 1)^2 = (x_1 x'_1 + x_2 x'_2 + 1)^2
\]

\[
= (x_1 x'_1)^2 + (x_2 x'_2)^2 + 2x_1 x'_1 x_2 x'_2 + 2x_1 x'_1 + 2x_2 x'_2 + 1
\]

\[
= [x_1^2, x_2^2, \sqrt{2} x_1 x_2, \sqrt{2} x_1, \sqrt{2} x_2, 1] [(x'_1)^2, (x'_2)^2, \sqrt{2} x'_1 x'_2, \sqrt{2} x'_1, \sqrt{2} x'_2, 1]^\top
\]

\[
\psi(x) = \psi(x')
\]

The projection \( \psi(x) \) defined this way spans the space of polynomials of degree 2 and has therefore dimensionality 6.

Polynomial kernels are all about the euclidian angle between two inputs. Additional, the euclidian length of both vectors play a role. If one likes to get rid of the last effect, a normalized polynomial kernel returns only the cosine between \( x \) and \( x' \) to the power of \( d \):

\[
k(x, x') = (\frac{x \cdot x'}{||x|| ||x'||})^d
\]

Different norms \( || \cdot || \) and parameters \( d \) and \( \sigma \) generate different kernels, which all imply an infinite dimensional RKHS [4]. The two most popular both use the \( L_2 \) norm and are called Laplacian \( (d = 1) \) and Gaussian \( (d = 2) \). The latter is by far the most common kernel and has become synonymous with the name RBF kernel.

**RBF kernels** A radial basis functions (RBF) kernel has the general form of

\[
k(x, x') = \exp \left( -\frac{||x - x'||}{\sqrt{2} \sigma} \right)^d.
\]

(2.15)

Different norms \( || \cdot || \) and parameters \( d \) and \( \sigma \) generate different kernels, which all imply an infinite dimensional RKHS [4]. The two most popular both use the \( L_2 \) norm and are called Laplacian \( (d = 1) \) and Gaussian \( (d = 2) \). The latter is by far the most common kernel and has become synonymous with the name RBF kernel.

RBF kernels are based on the distance of two input vectors. The kernel parameter \( \sigma \) determines the radius of influence for training samples. In well sampled regions (and well adjusted \( \sigma \)) the kernel shows good approximation properties but where no training data is available the kernels will produce only small output and therefore perform poorly.
CHAPTER 2. PRELIMINARIES

2.2.4 Kernelized covariance eigenvalue problem

Many unsupervised learning algorithms (e.g. PCA [8]) demand an eigenvalue decomposition of the covariance matrix:

\[
\text{cov}(X) = \mathbb{E}[xx^\top] - \mathbb{E}[x]\mathbb{E}[x]^\top = \frac{1}{n}XX^\top - \frac{1}{n^2}X11^\top X^\top = U_c\Lambda_c U_c^\top
\]  

(2.16)

In most cases one aims to project samples \( x \) onto eigenvectors \( U_c \):

\[
x' = U_c^\top x.
\]

To catch more complex, nonlinear relationships, one can expand \( x \) into a nonlinear feature space \( \psi(x) \). The kernel trick can help to describe the expansion more efficient (e.g. Kernel PCA [11]).

**Original approach** One starts with ensuring zero mean by subtracting the sample mean from all columns

\[
X_c = X - \frac{1}{n}X11^\top.
\]

Subsequently, one can perform the eigenvalue decomposition on the centered covariance matrix

\[
\frac{1}{n}X_cX_c^\top = U_c\Lambda_c U_c^\top.
\]

Standard implementations of eigenvalue decompositions have a complexity of \( O(p^3) \) with \( p \) being the dimensionality of samples \( x \).

**Inner and outer product** [8] If we want to reformulate the covariance matrix eigenvalue decomposition, we can exploit a relationship between the inner product \( X^\top X \) and outer product \( XX^\top \) of \( X \).

The singular value decomposition \( X = U\Sigma V^\top \) with \( \Sigma = [\Lambda_1^{1/2} \ 0] \) refers to eigenvalues and eigenvectors of both outer and inner product. Therefore, an eigenvalue decomposition of the inner product \( X^\top X = V\Lambda V^\top \) produces the same non zero eigenvalues \( \Lambda_r \) as the outer product and the corresponding eigenvectors \( U_r \) and \( V_r \) are related by:

\[
U_r = XV_r\Lambda_r^{-1/2}
\]  

(2.17)

**Kernelized approach** We proceed as before. With the Gram matrix of scalar products \( K = X^\top X \) at hand, we first have to center the data represented by it. Subtracting the sample mean \( X_c = X - \frac{1}{n}X11^\top \), it is easy to proof that the centered kernel matrix is:

\[
K_c = X_c^\top X_c = (I - \frac{1}{n}11^\top)K(I - \frac{1}{n}11^\top)
\]  

(2.18)

Secondly, we perform the eigenvalue decomposition \( K_c = V_c\Lambda_c V_c^\top \). Using (eq. 2.17) we can now express the term \( U_r^\top x \) with the nonzero eigenvalues \( \Lambda_r \) and corresponding eigenvectors \( V_r \) of \( K_c \):

\[
U_r^\top x = \sqrt{n}\Lambda_r^{-1/2}V_r^\top X^\top x
\]  

(2.19)

Replacing \( K \) by another kernel matrix \( \tilde{K} \) and the term \( X^\top x \) in (eq. 2.19) by \( \tilde{k}(x) \), we implicitly project the data into a feature space \( \psi(x) \) defined by the kernel:

\[
\tilde{U}_c^\top \psi(x) = \sqrt{n}\tilde{\Lambda}_r^{-1/2}\tilde{V}_r^\top \tilde{k}(x)
\]  

(2.20)
2.2. KERNEL TECHNIQUES

2.2.5 Kernel matrix approximation

The application of the kernel trick is restricted to a small amount of samples ($n \approx 5000 \ldots 10000$), because the kernel matrix stores $n \times n$ entries. If this number is exceeded, one would like to sacrifice approximation quality for manageable kernel matrix sizes. Different approaches have been made to overcome this problem by means of an approximation $\hat{K} \in \mathbb{R}^{m \times m}$ of the kernel matrix $K \in \mathbb{R}^{n \times n}$, where $m << n$ (see for example [10]). They all have in common that they assume a given subset of the training samples (support vectors) to be representative for the whole set.

An algorithm to select support vectors is presented in section 2.2.6.

Subset of Data [10] The simplest approach to kernel matrix approximation is called subset of data (SD). In this approach only the subset of $m$ support vectors is used and the approximation therefore has size $m \times m$. Because, only the support vectors influence $\hat{K}$ all information of the remaining $n - m$ samples is lost.

If the support vectors are chosen randomly out of the training set, subset of data is also known as the Nyström method [12].

Projected Process [10] A better suited approach is called projected process (PP). Here, the non support vector rows are removed but all columns are kept and the resulting matrix $\hat{K}$ has size $\mathbb{R}^{m \times n}$. The matrix $\hat{K} \hat{K}^\top \in \mathbb{R}^{m \times m}$ is used to approximate $K^2$. While preserving much more information, the method can only be applied to algorithms which use $K^2$.

This restriction can be circumnavigated, if an eigenvalue decomposition of $K$ has to be performed anyway. Because $K^2 = \mathbf{V} \Lambda^2 \mathbf{V}^\top$ for $K = \mathbf{V} \Lambda \mathbf{V}^\top$, it is sufficient to perform the eigenvalue decomposition on $\hat{K} \hat{K}^\top$. Taking the square root of the eigenvalues $\hat{\Lambda}$, together with the unchanged eigenvectors $\hat{\mathbf{V}}$, yields the projected process approximation of $K \approx \hat{\mathbf{V}} \hat{\Lambda}^{1/2} \hat{\mathbf{V}}^\top$.

2.2.6 Support vector selection

Whatever approximation method one chooses, the choice of support vectors is crucial to preserve as much information as possible. Selecting an optimal set of support vectors means to minimize a specific cost function with respect to the set of support vectors, which is a hard combinatorial problem [7].

A number of heuristics have been proposed to find a suitable set. Beside the purely random Nyström method [12], the sequential sparse Bayesian learning algorithm [6] (related to the relevance vector machine [3]) estimates the contribution of training samples to the optimization problem. The procedure works iteratively, but not greedy. For big training sets, the convergence is very slow. However, the method is specified for a Bayesian setting (like Gaussian processes [9], for example) and therefore not suitable for our purposes.
Algorithm 4 Greedy support vector selection algorithm

Require: $\nu, x^{(1)}, \ldots, x^{(n)}$

$SV_1 = \{x^{(1)}\}$

$K_i^{-1} = 1/k(x^{(i)}, x^{(1)})$

for $i = 2, \ldots, n$ do

$a_i = K_{i-1}^{-1}k(x^{(i)})$

$\epsilon_i = k(x^{(i)}, x^{(i)}) - k(x^{(i)})^T a_i$

if $\epsilon_i < \nu$ then

$SV_i = SV_{i-1} \cup \{x^{(i)}\}$

$K_i^{-1} = \frac{1}{\epsilon_i} \left[ \epsilon_i K_{i-1}^{-1} + a_i a_i^T - a_i a_i^T 1 \right]$ 

else

$SV_i = SV_{i-1}$

$K_i^{-1} = K_{i-1}$

end if

end for

return $SV_n$

In this thesis, we want to investigate another heuristic, which was proposed by Csató and Opper [13] and applied to a kernelized version of least square regression by Engel [14].

We assume the data $x$ to be mapped into a feature space $\psi(x)$, defined implicitly by a kernel $k(x, x') = \psi(x)^T \psi(x')$. Theorem 2.6 (representer theorem) assures that the optimal function is a linear combination of scalar products with training samples. If two expanded training samples would be linear dependent, omitting one would not change the optimal function. Likewise, those samples which can be approximated badly using linear combinations of the remaining set are likely to be important.

The idea of algorithm 4 is that for a given set of support vectors $SV = \{\tilde{x}^{(1)}, \ldots, \tilde{x}^{(m)}\}$, we define the approximated linear dependence (ALD) condition [14]:

$$\epsilon(x) = \min_a \left\| \sum_{j=1}^m a_j \psi(\tilde{x}) - \psi(x) \right\|^2 \leq \nu \quad (2.21)$$

where $\nu$ is an accuracy parameter determining the level of sparsity. The term $\epsilon(x)$ describes the minimal distance to the affine hull of set $SV$. It serves as an importance measure, which is independent of the problem we want to optimize afterwards.
When we denote the kernel matrix $K_{ij} = k(\tilde{x}^{(i)}, \tilde{x}^{(j)})$ and the kernel expansion $k(x) = [k(\tilde{x}^{(1)}, x), \ldots, k(\tilde{x}^{(m)}, x)]^\top$, we can express the left side of (eq. 2.21) as $\epsilon(x) = \min_a a^\top K a - 2a^\top k(x) + k(x, x) := \min_a L(x, a)$. The derivation with respect to $a$ yields:

$$\frac{\partial L(x, a)}{\partial a} = 2K a - 2k(x) = 0$$

$$a^* = K^{-1}k(x)$$

which allows us to reformulate the ALD condition (eq. 2.21):

$$\epsilon(x) = k(x, x) - k(x)^\top K^{-1}k(x) \leq \nu \quad (2.22)$$

All training samples $x$ for which (eq. 2.22) holds are considered "well approximated" and therefore omitted [14].

More precise, algorithm 4 runs sequentially through the training samples and tests if the current sample $x^{(i)}$ fulfills the ALD condition for the current set of support vectors $SV_{i-1}$. If the condition fails, the sample becomes a support vector and the inverse kernel matrix (which is guaranteed to be invertible for $\nu > 0$) is updated using the Woodbury matrix identity [9].

The overall complexity of the algorithm is $O(m^2)$ in space and $O(nm^2)$ in time.

The support vector set obtained by this method should be well-conditioned for most optimization problems. It also has the nice property that for every $\nu$ there is a maximum size for $SV_n$, which is independent of $n$.

**Proposition 2.7** Assume that (i) $k$ is a Lipschitz continuous Mercer kernel on $X$ and (ii) $X$ is a compact subset of $\mathbb{R}^d$. Then there exists a constant $C$ that depends on $X$ and on the kernel function such that for any training sequence $\{x^{(i)}\}_{i=1}^\infty$, and for any $\nu > 0$, the number of selected support vectors $N$, satisfies $N \leq C \nu^{-d}$.

**Proof:** See [14].

As a downside, the number of selected support vectors $m$ depends largely on input set $X$ and kernel $k(\cdot, \cdot)$. There is no way to estimate $m$ from the parameter $\nu$, which is responsible for the sparsity of $SV_n$. In practice one is interested in a support vector set of an appropriate (large but not too large) size. The experiments conducted in chapter 5 used RBF kernels and kept a fixed $\nu = 0.1$ while varying the kernel width $\sigma$. This procedure was repeated until a set of suitable size was found.
Chapter 3

Reinforcement Learning

In this chapter we will give an outline how to solve control problems (like robot navigation) with reinforcement learning. First, we will define the necessary terms of Markov decision processes (sec. 3.1.1), followed by a discussion of state space representation (sec. 3.1.2), especially trigonometric polynomials (sec. 3.1.3). Secondly, we will discuss linear algorithms for value (LSTD, sec. 3.2.1) and Q-value estimation (LSQ, sec. 3.2.2). Finally, we introduce the principles of policy iteration and present the least squares policy iteration (sec. 3.3) followed by a summarizing conclusion of the complete process (sec. 3.4).

3.1 Introduction

Learning behaviour for an autonomous agent means learning to choose the right actions at the right time. In machine learning, this is called a policy: A function that chooses an action based on some input representing the state of the world. In human terms, to define a policy we have to define two things first: The perception and the goal of the agent. The first defines what we see as a "state", the second what we see as "right".

While perception of the world is an open field which is mostly circumnavigated by defining some "essential variables" like position and orientation, behavioural experiments (classical conditioning, for example Pavlov’s dog bell) lead to a simple approach to the second question: Reward and punishment. In short, an agent should try to maximize his future reward while minimizing future punishment. Thus, training the agent becomes a simple choice what it shall and shall not do, eliminating the need to show it how.

Technically, we assume to have access to some function that filters meaningful (discrete or continuous) states out of the sensor data available to the agent. The exact nature of this function is of little importance to this chapter, besides that it provides the full state of the world. In this thesis, we want to show that Slow Feature Analysis (SFA, chapter 4) can learn such a function under
the right conditions.

The evolution of state and reward over time is modelled as a stochastic Markov decision process (MDP). Since a critical choice leading to reward or punishment might be necessary long before its fruits will be received, we can not use standard regression approaches. Instead we try to estimate future reward (punishment is simply negative reward) for all actions in a state and take the action which is most promising. The sum of the expected future reward is called value (sec. 3.2).

Unfortunately, the future (and with it the value) we are trying to predict for the policy, depends on the policy itself. Since this is a "hen or egg" problem, policy iteration methods repeat the steps value estimation and policy determination until they converge to the optimal policy which maximizes the value for all states (section 3.3).

3.1.1 Markov processes

After learning, we wish for the agent to move towards the reward. To do this, it has to learn which transition exist between a given set of states and where the reward is given. Once this knowledge is somehow established, it needs to find a decision function, telling it where to choose which action.

As we will see, the central element is the estimation of the sum of expected future rewards, called value. Value estimation is easiest in Markov reward processes (MRP), so we will start by introducing them to the reader. The MRP itself is unable to model control tasks, but there exists an extension named markov decision processes (MDP). MDP models the element of choice by introducing a set of actions between which a policy can choose. We will finish this section by defining the optimal policy, a function which chooses the action that will maximize the future reward.

**Definition 3.1 (Markov reward process MRP)** The discounted MRP $M = (S, P, R, γ)$ consists of a set of $n$ states $S = \{s_1, \ldots, s_n\}$, the transition probabilities $P : S \times S \rightarrow [0, 1]$ with $\forall s \in S : \sum_{i=1}^{n} P(s, s_i) = 1$, a function that assigns a real valued reward to every transition $R : S \times S \rightarrow \mathbb{R}$, and a discount factor $γ \in (0, 1]$.

MRPs are used to describe the statistical properties of the random walk of a variable $x \in S$ in discrete time steps and the reward it collects in the meantime. In opposition to iid drawing, the random walk is subject to the Markov property

$$P(x_t|x_{t-1}, \ldots, x_0) = P(x_t|x_{t-1}),$$

in other words the probability of being in state $x_t \in S$ at time $t$ depends exclusively on the predecessor state $x_{t-1} \in S$. In most situations reward depends solely on the outcome, so we simplify in the following $R : S \rightarrow \mathbb{R}$ as only dependent on the target state of a transition.
3.1. INTRODUCTION

Figure 3.1: A deterministic $16 \times 16$ states MRP (left) and the resulting value for $\gamma = 0.9$ (right). Arrows indicate the transition direction, entering $G$ is rewarded.

**Definition 3.2 (Value [22])** The value $V : S \to \mathbb{R}$ is the expected sum of future rewards, discounted by the factor $\gamma \in (0, 1]$:

$$V(x) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t R(x_{t+1}) \mid x_0 = x \right]$$

(3.2)

Due to the infinite sum, one commonly uses a recursive definition which is known as the Bellman function [22]:

$$V(x_t) = \mathbb{E} [R(x_{t+1}) + \gamma V(x_{t+1})] = \sum_{x' \in S} P(x_t, x') (R(x') + \gamma V(x'))$$

(3.3)

Intuitively, the value function $V(x)$ tells us which states are promising (figure 3.1). However, it does not say how to get there. For control purposes, we would need a function that returns the value of all possible actions in the current state. Within the framework of Markov decision processes, we can define exactly such a function, called $Q$-value.

**Definition 3.3 (Markov decision process MDP [27])** The discounted MDP $M = (S, A, P, R, \gamma)$ is an extension of the MRP to control problems. It defines an additional set of $m$ actions $A = \{a_1, \ldots, a_m\}$ and transition probabilities $P : S \times A \times S \to [0, 1]$ and reward function $R : S \times A \times S \to \mathbb{R}$ are extended to depend on the executed action as well.

As in the MRP case, we simplify the reward function as exclusively dependent on the target state: $\forall s \in S : R(s) = R(\cdot, \cdot, s)$.

**Definition 3.4 ((Stationary) Policy [27])** A function $\pi : S \times A \to [0, 1]$ with $\forall s \in S : \sum_{a \in A} \pi(s, a) = 1$ is called a stationary policy.

A policy represents a control or decision automat. $\pi(s, a)$ is the probability that the automat chooses action $a$ in state $s$. Since the value in a MDP depends
on future decisions, it is necessary that the policy is stationary (i.e. does not change) throughout value evaluation.

**Definition 3.5 (Q-value [27])** The Q-value $Q^\pi: S \times A \rightarrow \mathbb{R}$ of an MDP is the value of an action executed in a state, if all following actions are selected with respect to the stationary policy $\pi$:

$$Q^\pi(x_t, a_t) = \mathbb{E}[R(x_{t+1}) + \gamma Q^\pi(x_{t+1}, a_{t+1}) | x_{t+1} \sim P(x_t, a_t, \cdot), a_{t+1} \sim \pi(x_{t+1}, \cdot)]$$

$$= \sum_{x' \in S} P(x_t, a_t, x') \left( R(x') + \gamma \sum_{a' \in A} \pi(x', a') Q^\pi(x', a') \right)$$

(3.4)

The Q-value function defines implicitly a value function for every action (see figure 3.2). This way one can navigate by always choosing the action with the highest Q-value.

Of course, we can also reformulate the classical value function (eq. 3.3), which is now dependent on policy $\pi$, in terms of Q-values:

$$V^\pi(x_t) = \sum_{a \in A} \pi(x_t, a) Q^\pi(x_t, a)$$

(3.5)

**Lemma 3.1** For a given policy $\pi$, the value of a MDP $M = (S, A, P, R, \gamma)$ is equal to the the value of the MRP $M' = (S, P', R, \gamma)$ with $\forall s, s' \in S: P(s, s') = \sum_{k=1}^n \pi(s, a_k) P(s, a_k, s')$.

**Proof:** Insert (eq. 3.3) in (eq. 3.5). Together with the definition of $P'(s, s')$ one can derive (eq. 3.3). □

**Definition 3.6 (Optimal policy)** The optimal stationary policy $\pi^*$ maximizes the value $V^\pi(s)$ for every state $s \in S$:

$$\forall \pi, \forall s \in S: V^\pi^*(s) \geq V^\pi(s)$$

(3.6)

This is obviously the control function we were looking for. A control algorithm simply has to draw the actions according to $\pi^*$ and is guaranteed to find the best way to the reward. Lemma 3.2 shows how to define such a policy with the help of Q-values.
Lemma 3.2 (i) There can exist several \( \pi^* \) but (ii) at least one is equivalent to a deterministic selection function \( \alpha^* : S \to A \) with \( \forall s \in S : \pi^*(s, \alpha^*(s)) = 1 \):

\[
\alpha^*(s) = \arg \max_{a \in A} Q^\pi^*(s, a) \tag{3.7}
\]

Proof: (i) Consider \( a_1, a_2 \in A \) such that \( \max_a Q^\pi^*(s, a) = Q^\pi^*(s, a_1) = Q^\pi^*(s, a_2) \). For every \( \lambda \in [0, 1] \), the policy \( \pi(s, a_1) = \lambda, \pi(s, a_2) = (1 - \lambda) \) is optimal.

(ii) Due to (eq. 3.5) and (eq. 3.7), \( \forall s \in S : V^\pi^*(s) = \max_a Q^\pi^*(s, a) \). Therefore, \( \pi^* \) is optimal. \( \square \)

Of course, the Q-values them self depend on the policy and the only way to solve this dilemma is to improve both quantities in an alternating fashion (see policy iteration, section 3.3).

3.1.2 State representation

The MDP formalism provides us with a (possibly infinite) set of states \( S \). At this point we are interested in value estimation, that means we want to find a function \( v : S \to \mathbb{R} \) that at least approximates the value for all states. If we restrict ourselves to linear functions, i.e. \( v(x) = w^\top x \), we need a linear representation \( \phi : S \to \mathbb{R}^m \) to project the states into a subset of \( \mathbb{R}^m \).

Definition 3.7 (State representation) Let \( X \) be an arbitrary set. An injective function \( \phi : S \to X \) will be called a representation of the set of states \( S \). If \( X \subseteq \mathbb{R}^m \) for \( m \in \mathbb{N}^+ \), \( \phi \) will be called a linear representation.

We aim here to find a representation that works with linear functions, i.e. \( V^\pi^*(s) \approx v^\pi^*(\phi(s)) = w^\top \phi(s) \), in other words a linear representation. The injectivity of \( \phi \) guarantees that no two states have the same representation. Obviously the representation need additional properties to approximate a value function well. However, if \( S \) is a finite state space, there exists a representation that allows the exact approximation, i.e. \( V^\pi^*(s) = v^\pi^*(\phi(s)) \).

Definition 3.8 (Tabular representation [9]) The linear representation \( \phi : S \to \{0, 1\}^n \subset \mathbb{R}^n \) is called a tabular representation of \( S = \{s_1, \ldots, s_n\} \), if \( \forall i \in \{1, \ldots, n\} : \phi_i(s_i) = 1 \) and \( \forall j \neq i : \phi_j(s_i) = 0 \).

Lemma 3.3 The value function of every MRP or MDP can be exactly approximated as a linear function of a tabular representation (def. 3.8).

Proof: The linear function \( v^\pi(s) = w^\top \phi(s) \) with \( \forall i : w_i = V^\pi(s_i) \) represents the value \( V^\pi^*(s) \) exactly, since \( \forall i : v(s_i) = \sum_{j=1}^n w_j \phi_j(s_i) = w_i = V^\pi^*(s_i) \). \( \square \)

The size \( n \) of this representation is equal to the number of states. Since the value estimation algorithms we will discuss later have a complexity of \( O(n^3) \), this is not feasible for larger problems. Especially if we have a continuous, i.e. infinite state space, we are not able to approximate the value function exactly anymore.
Continuous state space  Due to the infinite number of states, we speak of the transition probability kernel $P(s,a,\cdot)$ and a reward function $R(\cdot)$ [33].

Instead of giving a formal derivation of continuous state spaces, we will restrict us to subsets of the euclidian space. Other spaces are imaginable, but euclidian subsets should cover most practical cases, from robot positions to pressure intensity.

**Assumption 3.9 (Compact subset [33])** The continuous state space $S$ is a compact subset of the $d$ dimensional euclidian space.

For example, the closed set of tuples that form the unit square $[0,1]^2$ is a compact subset of the 2-dimensional euclidian space.

The approximation quality of a linear function will depend entirely on the state representation $\phi$ and the value function at hand. The value will probably be continuous on most parts of a continuous state space, so it makes sense to choose a set of basis functions that are known to approximate continuous functions well. Examples are polynomials, splines [19] and trigonometric polynomials [18].

### 3.1.3 Trigonometric polynomials

In this thesis, trigonometric polynomials will play a major role, so we shortly introduce them here and discuss their approximative capabilities.

**Definition 3.10 (Trigonometric polynomial [20])** A trigonometric polynomial $T : \mathbb{R} \to \mathbb{R}$ of degree $d$ with the coefficients $a_0, \ldots, a_d$ and $b_1, \ldots, b_d$ is defined as:

$$T(x) = a_0 + \sum_{j=1}^{d} a_j \cos(2\pi j x) + \sum_{j=1}^{d} b_j \sin(2\pi j x) \quad (3.8)$$

Maybe the most famous trigonometric polynomial (of degree $d \to \infty$) is the *Fourier series* [20]. Trig. polynomials of degree $d$ are a linear combination of the first $2d + 1$ trigonometric basis functions $\psi(x)$:

$$\forall j \in \mathbb{N} : \psi_j(x) = \begin{cases} 
\cos(j \pi x) & \text{j even} \\
\sin((j + 1) \pi x) & \text{j odd}
\end{cases} \quad (3.9)$$

So we can express every trig. polynomial of degree $d$ as $T(x) = \sum_{i=0}^{2d} w_i \psi_i(x)$. However, most continuous state spaces will be multidimensional.
Definition 3.11 (Multivariate trigonometric polynomial) A multivariate trigonometric polynomial $T: \mathbb{R}^p \rightarrow \mathbb{R}$ of degrees $d_1, \ldots, d_p$ in the respective input dimensions, with the coefficients $w \in \mathbb{R}^m$ and $m = \prod_{n=1}^{p} (2d_p + 1)$ is defined as:

$$T(x) = \sum_{n_1=0}^{2d_1} \ldots \sum_{n_p=0}^{2d_p} w_{\mu(n_1, \ldots, n_p)} \prod_{k=1}^{p} \psi_{n_k}(x_k)$$

(3.10)

$$\mu(n_1, \ldots, n_p) = \sum_{i=1}^{p} \left( n_i \prod_{j=i+1}^{p} (2d_j + 1) \right), \quad \text{(index function)} \quad (3.11)$$

Intuitively spoken, the multivariate trig. polynomial is the weighted sum of all combinations of trigonometric basis functions in all input dimensions.

Definition 3.12 (Trigonometric representation) The linear representation $\phi: S \rightarrow \mathbb{R}^m$ of the continuous state space $S = [-1,1]^p \subset \mathbb{R}^p$ called trigonometric representation with degrees $d_1, \ldots, d_p$ and $m = \prod_{n=1}^{p} (2d_p + 1)$ is defined as:

$$\forall i \in \{1, \ldots, p\} : \forall n_i \in \{1, \ldots, d_i\} : \phi_{\mu(n_1, \ldots, n_p)}(x) = \prod_{k=1}^{p} \psi_{n_k}(x_k)$$

(3.12)

Thus, we can express every multivariate trig. polynomial as a linear function with a trig. representation of the same degree: $T(x) = \sum_{i=1}^{m} w_i \phi_i(x)$.

Theorem 3.4 ([18], Thm 4.25) For every continuous function $f: \mathbb{R}^p \rightarrow \mathbb{R}$ and every $\epsilon > 0$, there is a trigonometric polynomial $T(x)$, such that $\forall x \in [-1,1]^p : |f(x) - T(x)| < \epsilon$.

Proof: See [18].

This theorem states that we can approximate any continuous function pointwise arbitrary well as a multivariate trigonometric polynomial.

However, since we are initially unaware of the the value function, we have to pick the degrees before the estimation. This leaves us with the question how big the estimation error will be for given degrees $d_1, \ldots, d_p$. One can expect that it is related to the smoothness of the value function at hand, which strictly does not even have to be continuous (e.g. at walls). See Lorentz [17] for details.
3.2 Value Estimation

In this section we want to present algorithms to estimate value and Q-value functions. Instead of giving a complete overview of the topic, we want to restrict us to model free approaches, because for control purposes we are only interested in the Q-value, anyway.

We understand under model free value estimation the absence of an explicit model of the MDP, i.e. $P(\cdot, \cdot, \cdot)$ and $\pi(\cdot, \cdot)$. Also, the state space $S$ and reward function $R(\cdot)$ does not need to be known. However, we explicitly need to know action space $A$ and discount factor $\gamma$. Of course, there also exist explicit model approaches for value estimation. For example in [34] independent models of the transition matrix and the reward function were learned. It is also shown that for linear models their approach yields exactly the same solution as a model free approach.

Because of these restrictions, we can only minimize the Bellman error

$$BE(\hat{V}) = \mathbb{E}[R_t + \gamma \hat{V}(x'_t) - \hat{V}(x_t)]$$

over a set of transitions $x_t \rightarrow x'_t$ with reward $R_t$.

In this thesis, we only consider the case of linear function classes as estimation model. The standard approach is called temporal difference learning. Classic algorithms like $TD(\lambda)$ and Monte Carlo [21] are left out for the benefit of least squares temporal difference algorithms. These circumnavigate a number of problems of classical algorithms we can not go into detail here.

3.2.1 LSTD

The least squares temporal difference (LSTD) algorithm estimates value functions of MRP and was first developed by Bradtke and Barto [22]. Later, in line with the extension of $TD$ to $TD(\lambda)$, the algorithm was extended to LSTD($\lambda$) by Boyan [24]. We will discuss the original LSTD algorithm, but in a formalism that resembles Boyans extension.

LSTD is defined on MRP, so we assume a training set $T = \{(\phi(x_i), r_i, \phi(x'_i))\}_{i=1}^n \subseteq (\mathbb{R}^m \times \mathbb{R} \times \mathbb{R}^m)$ of $n$ transitions $x_t \rightarrow x'_t$ with reward $r_t$. The sampling of $x_t$

| Algorithm 5 LSTD |
|------------------|
| **Require:** $\gamma$; $\{(\phi(x_i), R_i, \phi(x'_i))\}_{i=1}^n \subseteq (\mathbb{R}^m \times \mathbb{R} \times \mathbb{R}^m)$ |
| $A_0 = \text{zeros}(m,m)$ |
| $b_0 = \text{zeros}(m,1)$ |
| for $i = 1, \ldots, n$ do |
| $A_i = A_{i-1} + \phi(x_i)(\phi(x_i) - \gamma \phi(x'_i))^T$ |
| $b_i = b_{i-1} + \phi(x_i)R_i$ |
| end for |
| $w = \text{pinv}(A_n)b_n$ |
| return $w$ |
3.2. VALUE ESTIMATION

affects the solution and should be as uniform as possible. The states can be represented by an arbitrary injective function \( \phi : S \rightarrow \mathbb{R}^m \).

For readability, we define the matrices \( \Phi_{ij} = \phi_i(x_j) \) and \( \Phi'_ij = \phi_i(x'_j) \).

**Optimization problem** LSTD minimizes a cost function related to the Bellman error [22]:

\[
C_{lstd}(w, (\Phi, \Phi', R)) = \frac{1}{n} \left\| \Phi (\Phi - \gamma \Phi')^\top w - \Phi R \right\|_F^2
\]

(3.14)

with the linear function \( \hat{V}^\pi(x) = w^\top \phi(x) \) and \( \mathbb{E}_t[\cdot] \) being the empirical mean.

Deriving (eq. 3.14) with respect to \( w \) yields the minimum \( w^* \):

\[
\frac{\partial C_{lstd}(w, (\Phi, \Phi', R))}{\partial w} = \frac{2}{n} \Phi \gamma \Phi^\top \Phi \Phi^\top w - \frac{2}{n} \Phi \gamma \Phi^\top \Phi R \equiv 0
\]

\[
\Rightarrow w^* = (\Phi \gamma \Phi^\top \Phi \Phi^\top)^{-1} \Phi \gamma \Phi^\top \Phi R
\]

where \( \Phi \gamma = \Phi - \gamma \Phi' \) and \( \dagger \) denotes the pseudo inverse. The last line holds if the rows of \( \Phi \Phi^\top \gamma \) are linearly independent [24].

LSTD (algorithm 5) has a complexity of \( O(m^2) \) in space and \( O(m^3) \) in time with \( m \) being the length of the state representation.

### 3.2.2 LSQ

The least squares Q-value (LSQ) algorithm was introduced by Lagoudakis et al. [26] to extend LSTD to Q-values. The basic idea is an extension of the state representation \( \phi : S \rightarrow \mathbb{R}^m \) to state action representation \( \phi : S \times A \rightarrow \mathbb{R}^m \).

**Definition 3.13 (State action representation [26])** An arbitrary linear representation \( \phi : S \rightarrow \mathbb{R}^m \) (e.g. of a continuous state space) can be extended by a discrete set of actions \( A = \{a_1, \ldots, a_k\} \) to a combined representation \( \phi : S \times A \rightarrow \mathbb{R}^{mk} \) with \( \forall s \in S, \forall a_i \in A : \phi(s, a_i) = [z_a^\top, \phi(s)^\top, z_b^\top]^\top \), \( z_a \in \{0\}^{(i-1)n} \) and \( z_b \in \{0\}^{(m-i)n} \).

**Algorithm 6 LSQ**

Require: \( \phi : S \times A \rightarrow \mathbb{R}^m \); \( \gamma; \{x_i, a_i, R_i, x'_i, a'_i\}_{i=1}^n \subset (S \times A \times \mathbb{R} \times S \times A) \)

for \( i = 1, \ldots, n \) do

\( \phi_i = \phi(x_i, a_i) \)

\( \phi'_i = \phi(x'_i, a'_i) \)

end for

\( w = \text{LSTD}(\gamma; \{(\phi_i, R_i, \phi'_i)\}_{i=1}^n) \)

return \( w \)
Formally, we assume a training set \( \mathcal{T} = \{(x_i, a_i, R_i, x'_i, a'_i)\}_{i=1}^{n} \) of \( n \) observed transitions \( x_i \xrightarrow{a_i} x'_i \), the collected reward \( R_i \) and the next action \( a'_i \) chosen according to \( \pi \). The states might be available in an additional representation, but they serve only as input for \( \phi(\cdot, \cdot) \).

**Proposition 3.5** Given a stationary policy \( \pi \) and a state action representation \( \phi : S \times A \rightarrow S' \), the Q-value \( Q^\pi(s, a) \) of the MDP \( M = (S, A, P, R, \gamma) \) is equal to the value \( V'(\phi(s, a)) \) of the MRP \( M' = (S', P', R', \gamma) \), where

\[
\forall s, s' \in S, \forall a, a' \in A:\n\begin{align*}
(i) & \quad S' = \bigcup_{s \in S} \bigcup_{a \in A} \{\phi(s, a)\} \\
(ii) & \quad P'(\phi(s, a), \phi(s', a')) = P(s, a, s')\pi(s', a') \\
(iii) & \quad R(\phi(s, a), \phi(s', a')) = R(s, a, s')
\end{align*}
\]

**Proof:** \( \forall s \in S, \forall a \in A: \)

\[
Q^\pi(s, a) = \sum_{s' \in S} P(s, a, s') \left( R(s, a, s') + \gamma \sum_{a' \in A} \pi(s', a') Q^\pi(s', a') \right) \\
= \sum_{s' \in S} \sum_{a' \in A} \left( \pi(s', a') P(s, a, s') R(s, a, s') + \gamma P(s, a, s') \pi(s', a') Q^\pi(s', a') \right) \\
= \sum_{s' \in S} \sum_{a' \in A} P'(\phi(s, a), \phi(s', a')) \left( R(\phi(s, a), \phi(s', a')) + \gamma V'(\phi(s', a')) \right) \\
= V'(\phi(s, a))
\]

The last equality holds only if \( \phi(\cdot, \cdot) \) is injective. \( \square \)

LSQ combines the state and action using a injective function \( \phi(\cdot, \cdot) \) (e.g. definition 3.13), and then utilizes LSTD to estimate \( V'(\phi(\cdot, \cdot)) \). Since no explicit model of the MDP is needed, estimating \( V'(\phi(\cdot, \cdot)) \) is an easy way to estimate \( Q^\pi(\cdot, \cdot) \). The policy affects the solution through \( a'_i \sim \pi(x'_i, \cdot) \), which satisfies definition 3.5 (Q-values).

### 3.3 Policy Iteration

With lemma 3.2, we have found an intuitive way to realize the optimal policy by means of Q-values. These can be estimated model free by the LSQ algorithm (sec. 3.2.2). However, the training set is sampled using a (not necessary known) policy and LSQ needs a policy to choose \( a' \).

A solution to this problem is called **policy iteration** and consists of a sequence of monotonically improving policies \( \pi_0, \ldots, \pi_m \) of the form \( [21] \):

\[
\alpha_i(s) = \arg \max_a Q^{\pi_i}(s, a) \\
\forall s \in S : \pi_{i+1}(s, \alpha_i(s)) = 1 \quad (3.15)
\]

The evaluation of \( \pi_m \) obviously requires an iterative alternation of Q-value estimation of policy \( \pi_i \) and policy improvement (eq. 3.15) to achieve a so called **greedy policy** \( \pi_{i+1} \). For the initial policy \( \pi_0 \), one often chooses a random policy with equal probabilities for all actions.
3.3. POLICY ITERATION

Algorithm 7 LSPI

 Require: $\phi : S \times A \to \mathbb{R}^m$; $\gamma$; $\epsilon$

 Generate $\{x_i, a_i\}_{i=1}^n \subset S \times A$ uniformly distributed

 Measure all $x'_i$ and $r_i$ in experiments based on $x_i$ and $a_i$

 Generate all $a'_i$ uniformly distributed for initial random policy

 // Policy iteration

 $w = \infty$; $w' = 0$

 while $||w - w'|| \geq \epsilon$ do

 $w' = w$

 $w = \text{LSQ}(\phi; \gamma; \{x_i, a_i, r_i, x'_i, a'_i\}_{i=1}^n)$

 for $i \in \{1, \ldots, n\}$ do

 $a'_i = \arg\max_a (w^\top \phi(x'_i, a))$

 end for

 end while

 return $w$

In the case of tabular state representation it is possible to prove the monotonic improving property of policy iteration. Approximations of $Q^\pi$, however, complicate convergence proofs and depend on approximation quality and Q-value estimation algorithm [27].

3.3.1 Sampling

For estimating Q-values, we need a training set $T = \{(x_i, a_i, r_i, x'_i, a'_i)\}_{i=1}^n \subset S \times A \times \mathbb{R} \times S \times A$. All $x'_i \sim P(x_i, a_i, \cdot)$ and $r_i \sim R(x_i, a_i, \cdot)$ follow the MDP and all $a'_i \sim \pi_j(x'_i, \cdot)$ are drawn according to the current policy. The start states $x_i$ and actions $a_i$, however, have to be sampled by another process.

Most experiments are performed in trajectories. For every trajectory of length $l \in \mathbb{N}^+$ we draw a start state according to some distribution $\hat{s}(\cdot)$ and follow a stationary policy $\hat{\pi}$, i.e. $\forall i \in \{1, \ldots, l\}: x_i = x'_{i-1}, a_i \sim \hat{\pi}(x_i, \cdot)$.

However, this approach can lead to some obstacles that can ruin the convergence of policy iteration. We will demonstrate the problem on a simple version of the Sarsa algorithm [23] and the solution with the LSPI algorithm [26].

Sarsa The easiest approach is to record a number of trajectories with a uniform start distribution $\hat{s}$ and to follow the current policy, i.e. $\hat{\pi} = \pi_i$.

Since equation 3.15 is based on the maximum of $Q^\pi(s, \cdot)$ in a state $s \in S$, it is necessary that $Q^\pi(s, a)$ is approximated well for all $a \in A$. This is not the case here, since every policy but the first is greedy. Sarsa will therefore choose the same action every time it visits the same state. This will lead to a poor approximation of all but the currently preferred action and therefore to poor policy convergence.

To be precise, in [23] Sarsa chooses actions $\epsilon$-greedy, i.e. with a (iteration dependent) probability of $\epsilon$ greedy and with $(1 - \epsilon)$ random.
Algorithm 8 Control

Require: $\phi : S \times A \rightarrow \mathbb{R}^m$; $w^*$

while true do
    $x = \text{observe}()$
    $a = \arg \max_a (w^* \phi(x, a))$
    $\text{execute}(a)$
end while

LSPI It is therefore important to draw $a_i$ as well as $s_i$ randomly, uniform distributed at best [27]. One way to achieve this is to record an initial dictionary with a random policy $\tilde{\pi}$ and change only $a'$ between the iterations. This approach is called least squares policy iteration and ensures equally well approximated Q-values.

On the one hand, this approach eliminates the need for resampling every iteration, which reduces the experimental overhead. On the other hand, there is no way to compensate unbalanced sampling in the dictionary. A random walk constrained by a complex environment can be very erratic, especially with few but long trajectories. Optimally, one would record trajectories of length 1 with $\tilde{s}$ and $\tilde{\pi}$ being uniform distributions over $S$ and $A$, respectively.

Algorithm 7 shows the complete LSPI method, for more information see [26] and [27].

3.4 Conclusion

In this chapter we presented an outline how to solve control problems with reinforcement learning.

- Algorithm 8 shows how the control works after an optimal policy, represented by the parameter vector $w^*$, is obtained by LSPI.

- For LSPI (alg. 7), it is sufficient to record one random walk to train the complete control procedure. To fulfill LSPIs requirement of uniformly distributed start states and actions, one can rely on the original random walk properties (given enough examples) or sample a balanced set out of the video to create a dictionary.

- Using LSQ (alg. 5) and LSTD (alg. 4) we can estimate the Q-value without knowledge of the underlying MDP. Only some samples in the dictionary have to be labeled as reward or punishment.

- The states can be given in any representation, if we use definition 3.13 to generate state action representations. However, a representation suited for linear functions is recommendable, e.g. a trigonometric representation (def. 3.12).
Chapter 4

Slow Feature Analysis

In this chapter we want to introduce an unsupervised learning criteria called slow feature analysis (SFA, sec. 4.1.1). SFA is used to find continuous states in temporal data. As a big advantage, theoretical tools are available that predict the behaviour in a variety of situations (sec. 4.1.2). We give an overview of recent applications in section 4.2 and conclude with the commonly used linear SFA algorithm (sec. 4.3.1). Since linear SFA is not suited for the task in this thesis, we also develop a kernelized version of the linear SFA algorithm (sec. 4.3.3).

4.1 Introduction

Biological systems start with little hard-coded instructions (e.g. genes). They grow, however, far more complex over time. It is estimated that the human genome consists of approximately 25,000 genes; the human brain alone is composed of $10^{11}$ neurons, each with its own individual properties. Therefore, biological systems must have a way of self-organizing and diversification, depending on the environment.

To understand and reproduce this learning-without-a-teacher, the field of unsupervised learning was developed. In contrast to supervised learning (e.g. regression, section 2.1) no target value is available, thus the design of the cost function alone determines the optimal function. Since there is no explicit target, every optimization problem has to rely on a self-organizing principle.

Temporal coherence The underlying principle of slow feature analysis are temporal coherent signals.

Imagine a sensor of undetermined type. All we can see are the multidimensional sensor readings, which probably are distorted by some kind of uncorrelated noise. Whether the sensor itself is moved or the environment changes around it, the readings will vary over time. We are searching for a filter which...
applied on the sensor readings yields a meaningful representation of the current state of environment.

As shortly addressed in the last chapter (sec. 3.1), there is no mutual consent what exactly a state of the environment is. The approach taken here is to concentrate on the things changing over time. For example, if an object is moved in front of a static background, than the background (as complex as it might be) is completely irrelevant for the state. The object, however, is equally unimportant. Only its position varies over time, and is therefore the state of the environment.

Keeping in mind that noise is considered uncorrelated to the state and therefore not markovian, a filter specializing on noise will change quickly. On the other hand, most important things in the real world change slowly and continuously over time. Therefore we should look for filters that produce a slowly varying output, while making sure that they vary at all and not just represent background. Because the state of something as complex as a real environment must be multidimensional, we should expect a set of filters, which have to be independent of each other. This means at least they have to be decorrelated.

State spaces extracted with such a filter will be temporal coherent, but ignore fast changing processes, e.g. the ball in table tennis.

4.1.1 Optimization problem

There are several approaches to learn a filter as described above. They share some basic claims on the filters output which were formulated best by Wiskott et al. [35, 37].

- The mean temporal derivation of the output should be as small as possible. Normally the derivation is not known, so the discrete temporal derivation, i.e. the difference between successive outputs, is used instead. To punish large changes more than small ones, all approaches square the derivation pointwise. This value is called slowness.

- To ensure that the output varies at all, the variance of the output is normalized, either by constraint or by multiplying the cost function with the inverse variance. This claim is equivalent to a zero mean and unit variance constraint.

- The different filters should be independent of each other. Since statistical independence is hard to achieve, all sighted works restrict themself to claim decorrelation between the filters.
4.1. INTRODUCTION

Definition 4.1 (SFA Problem [35])

Given a temporally ordered sequence of observations \(x^{(1)}, \ldots, x^{(n)} \in X\), we want to find a set of \(k\) mappings \(\phi_i(x) : X \to \mathbb{R}\) that satisfy:

\[
\begin{align*}
\min \ s(\phi_i) & := \mathbb{E}[\dot{\phi}_i(x)^2] \quad \text{(slowness)} \\
\text{s.t. } \mathbb{E}[\phi_i(x)] &= 0 \quad \text{(zero mean)} \\
\mathbb{E}[\phi_i(x)^2] &= 1 \quad \text{(unit variance)} \\
\forall j \neq i : \mathbb{E}[\phi_i(x)\phi_j(x)] &= 0 \quad \text{(decorrelation)}
\end{align*}
\]

where \(\dot{\phi}\) denotes the temporal derivative and \(s(\phi_i)\) the slowness of mapping \(\phi_i\). The indices \(i\) are sorted in ascending order according to their slowness, so the first mapping is the slowest.

Grouping the outputs and its discrete derivatives into matrices \(\Phi_{it} = \phi_i(x^{(t)})\) and \(\dot{\Phi}_{it} = \phi_i(x^{(t+1)}) - \phi_i(x^{(t)})\) we can express problem 4.1 more compact:

\[
\begin{align*}
\min \ s(\Phi) &= \text{tr}(\dot{\Phi}^\top \Phi) \\
\text{s.t. } \Phi 1 &= 0 \\
\Phi \Phi^\top &= I
\end{align*}
\] (4.1)

Other approaches

Besides Wiskott et al. [35], we found two other optimization problems that follow the principle of temporal coherence:

- Bray and Martinez [36] formulated as a related cost function the ratio of long- and short-term variance \(V\) and \(S\):

\[
\max F(\Phi) = \frac{V}{S} = \frac{\mathbb{E}[\phi(x)^2]}{\mathbb{E}[\dot{\phi}(x)^2]} \tag{4.2}
\]

where \(\phi(x)\) and \(\dot{\phi}(x)\) are the centered long- and short-term means, e.g. \(\bar{\phi}_i(x^{(t)}) = \frac{1}{2m} \sum_{j=t-m}^{t+m-1} \phi_i^{(j)}\) and an equivalently defined \(\bar{\phi}\) with smaller \(m\).

Minimizing the short term change (derivation) while maximizing the long term change (variance) follows the same principle as SFA. Decorrelation, however, is not required by this optimization problem and only appears in the results of [36], because the problem is solved with an eigenvalue decomposition, for which the solution is decorrelated by default.

- Einhäuser et al. [40] used a cost function which is based on the same constraints but was formulated differently:

\[
\max F(\Phi) = -\sum_{i=1}^{k} \frac{\mathbb{E}[\phi_i(x)^2]}{\sqrt{\mathbb{E}[\phi_i(x)^2]}} - \frac{1}{(k-1)^2} \sum_{i=1}^{k} \sum_{j \neq i}^{k} \frac{\mathbb{C}[\phi_i(x), \phi_j(x)]^2}{\sqrt{\mathbb{V}[\phi_i(x)]} \sqrt{\mathbb{V}[\phi_j(x)]}} \tag{4.3}
\]

The first term on the right side incorporates the minimization of the slowness with the unit variance constraint, the second term represents the decorrelation constraint.

\(^1\) The presented formalism is no direct citation but a readable version.
Wyss et al. [41] used a weighted version of this cost function with an additional zero mean constraint embedded the same way.

4.1.2 Optimal responses

Consider we could solve problem 4.1 in the class of continuous functions. Since the form of the optimal function depends on the training sequence at hand, we are interested in the form of the output, which should always be the same.

Definition 4.2 (Optimal responses) Let $O$ be an unsupervised optimization problem based on samples from set $X$. Let further $f$ be the optimal function of $O$ based on any infinite training set $T \subset X$. Then $\{ f(x) | x \in T \}$ is called the optimal responses of $O$.

In our case, we look for the function that describes the slowest output that still fulfills the constraints of problem 4.1. One can use variational calculus to find a solution independent of a specific input. [37].

Formally we assume some stochastic process that generates the training set. The process consists of a state in a bounded and continuous state space $S$ and some generating parameters, e.g. a position $s \in [0, 1] \subset \mathbb{R}$ plus a Gaussian random variable: $s^{(t+1)} = s^{(t)} + N(0, \sigma)$. $s$ would be the state and $\sigma$ the velocity of change. A function $\nu : S \to X$ generates observations $x \in X$ out of the true states.

There have to be some rules that constraint the stochastic process to $S$. The optimal responses will depend on what happens if a boundary is reached, i.e. if the state is stopped (reflected) or continues at the opposite boundary. These rules are incorporated into the variational calculus approach by boundary conditions.

Proposition 4.1 A set of functions which applied on a training sequence fulfills zero mean, unit variance, decorrelation and has orthogonal time derivatives, minimizes problem 4.1 within the space spanned by these functions.

Proof: See [37].

This proposition essentially gives us the means to validate a proposition about optimal responses. We start with the simple case of a compact subset of the one dimensional Euclidean space. Without loss of generality, assume $S = [0, 1]$. 

4.1. INTRODUCTION

Proposition 4.2 (Cyclic boundary condition) Assuming a cyclic boundary condition, i.e. \( \nu(0) = \nu(1) \), the optimal responses are \( \forall x \in [0, 1], \forall i \in \mathbb{N}^+ : \)

\[
\phi_i^*(\nu(x)) = \begin{cases} 
\sqrt{2} \cos(j \pi x) & \text{if } i \text{ even} \\
\sqrt{2} \sin((j + 1) \pi x) & \text{if } i \text{ odd}
\end{cases} \tag{4.4}
\]

Proof: Proposition 4.1 holds. See [37] for details.

Any cyclic state, e.g. orientation or electrical phase, is subject to this condition. Note the similarity to trigonometric basis functions (eq. 3.9), i.e. with the exception of the constant \( \psi_0 \), all basis functions are present. The domain, however, is only \([0, 1]\) instead of \([-1, 1]\), reflecting the cyclic boundary constraint.

Proposition 4.3 (Free boundary condition) Assuming no boundary condition, the optimal responses are \( \forall x \in [0, 1], \forall i \in \mathbb{N}^+ : \)

\[
\phi_i^*(\nu(x)) = \sqrt{2} \cos(j \pi x) \tag{4.5}
\]

Proof: Proposition 4.1 holds. See [37] for details.

Any state between two limits, e.g. coordinates restricted by walls, is subject to the free boundary condition. In fact, this is another expression of the trigonometric polynomial on the interval \([0, 1]\) instead of \([-1, 1]\). Since the even trig. basis functions can approximate any even continuous function in the interval \([-1, 1]\), they can approximate any continuous function in \([0, 1]\) [37].

However, many realistic scenarios require multidimensional state spaces. For example, a robot who can move freely on a plane and look in any direction, requires a 3-dimensional space. Franzius et al. [42] derived a solution for this case. They considered a stochastic generation process where an agent (e.g. a robot) can move in the direction it faces and rotate to change this direction. This implies a state space \( S = [0, 1]^3 \), where the first two directions represent two spatial degrees of freedom and the last the orientation, all scaled to the interval \([0, 1]\).

Proposition 4.4 (3d state space) Let \( S = [0, 1]^3 \) be a state space with free boundary conditions in the first two, and a cyclic boundary condition in the last dimension. Under the condition of decorrelated movements in the training set, the optimal responses are \( \forall x, y, \theta \in [0, 1] : \forall (i, j, l) \in \mathbb{N}^3 \setminus \{(0, 0, 0)\} : \)

\[
\phi_{ijl}^*(\nu(x, y, \theta)) = \begin{cases} 
\sqrt{2} \cos(i \pi x) \cos(j \pi y) \cos(l \pi \theta) & \text{if } i \text{ even} \\
\sqrt{2} \cos(i \pi x) \cos(j \pi y) \sin((l + 1) \pi \theta) & \text{if } i \text{ odd}
\end{cases} \tag{4.6}
\]

Proof: Proposition 4.1 holds. See [42] for details.

The solution resembles the trigonometric representation (def. [36, 42]), but uses the basis functions of the one dimensional boundary cases instead of \( \psi \).

However, these analytical solutions are exceptions. Experiments show that non-rectangular state spaces of the same dimensionality develop different optimal responses (sec. [5, 26]).
Proposition 4.5 (Mixture responses) If \( \phi_i \) and \( \phi_j \) are two optimal functions of problem 4.1 with equal slowness, then any linear combination \( a\phi_i + b\phi_j \) has the same slowness, as long as \( a^2 + b^2 = 1 \).

Proof: 

\[
\begin{align*}
\mathbb{E}(a\phi_i(x) + b\phi_j(x))^2 & = a^2\mathbb{E}[(\dot{\phi}_i(x))^2] + 2ab\mathbb{E}[\dot{\phi}_i(x)\dot{\phi}_j(x)] + b^2\mathbb{E}[(\dot{\phi}_j(x))^2] \\
& = a^2\mathbb{E}[(\dot{\phi}_i(x))^2] + 2ab\mathbb{E}[\dot{\phi}_i(x)\dot{\phi}_j(x)] + b^2\mathbb{E}[(\dot{\phi}_j(x))^2] \\
& = a^2s(\phi_i) + b^2s(\phi_j) \quad (\text{Prop. 4.1})
\end{align*}
\]

Therefore, we have to expect mixture responses between all filters of equal slowness. Note that this does not change the number of decorrelated filters, only their output is no longer determined by proposition 4.4.

4.2 Applications

To the authors' knowledge, there are no practical applications based on slow feature analysis. There are, however, a couple of scientific works that investigate its potential in different contexts.

4.2.1 Receptive fields

The first brain area processing visual information from the eye is called visual cortex. It contains cells that specialize on specific patterns (e.g., bars of specific orientation) in a small part of the perceived image, a so-called receptive field. The question arises how these cells differentiate and adopt patterns that allow an efficient coding of the perceived scene.

Berkes and Wiskott [38] used SFA to learn filters that react on patterns similar to those of real cells. They constructed a random process that moved a frame over natural pictures by translation, rotation and/or zooming (fig. 4.1a). Input samples consisted of two successive frames to represent a special neuronal structure called complex cells (fig. 4.1b). The results (fig. 4.1c) resemble phase shifted gabor filters, as they are found in these cells.

The results build a convincing argument, but for the sake of completeness one has to add that there are other unsupervised methods that produce similar filters. For example, Lindgren and Hyvärinen used quadratic ICA and also produced comparable results, though in a smaller resolution [43].
4.2. APPLICATIONS

4.2.2 Pattern recognition

Naturally SFA predicts continuous states. While discrete states (e.g., classes of patterns) present no problem in principle, the absence of a temporal structure is.

Berkes constructed a classifier for handwritten digits from the MNIST database based on SFA [39]. Instead of a temporal derivative, two training digits of the same class were subtracted, thus minimizing the distance between alike patterns. For the final classification, Gaussian distributions were fitted to the digit classes, each representing the probability of membership.

With 1.5% error rate on a test set of 10,000 samples, the specified classifier performed comparable to established algorithms in this field, e.g., the LeNet-5 algorithm misclassified 0.95% of the test set in comparison to 12% by a linear classifier.

4.2.3 Place cells

Rodents are known to develop specialized place cells in hippocampal areas after familiarizing themselves with their surroundings. These cells are only active in one part of the room, independent of the head’s orientation (fig. 4.6a). Together with head-direction cells, for which the output depends only on the orientation, independent of the rodents’ position, they are believed to play a major role in the rodents’ sense of navigation [42].

Franzius et al. [42, 44] developed a system that exhibits place and head-direction cell-like characteristics by applying SFA to the video of a virtual rat’s random walk. First, the random walk of a virtual rat in a rectangular room...
(fig. 4.3a) was recorded with a virtual wide angle camera mounted on the head (fig. 4.3b). The single frames were segmented in overlapping patches (nodes in fig. 4.3c) in line with the concept of receptive fields. SFA was performed on all patches, then the output was rearranged to overlapping receptive fields of the next layer, and so forth. This way the multi-layer network was able to cope with the high dimensional video input, despite the fact that linear SFA (sec. 4.3.1) with a quadratic expansion (sec. 4.3.2) of the patches was used for layer wise training (fig. 4.3d).

By using a suitable (i.e. powerful enough) function class in the SFA training, the output of the last layer has to resemble the theoretical predictions of proposition 4.4. Since the mean rotational and translational velocity of the rat influences the slowness of the optimal responses $s(\phi_{ijl})$ and therefore their ordering, it is possible to extract orientation or location invariant features by controlling the random walk. Slow movements with fast rotations lead to orientation invariance in the first SFA filters (fig. 4.4). Slow rotations and fast movements, on the other hand, will produce position invariance.

If we want to derive place cells, higher SFA filters are useless. The first orientation dependent filter $\phi_{001}$ will mix with all orientation invariant filters of equal slowness, so the mixed output will not be invariant to orientation anymore. Therefore, the virtual rat moved slow and rotated fast to obtain the results in figure 4.3.

The last step of Franzius et al. (fig. 4.3c) was the application of independent component analysis (ICA, [2]) on the last layers output. The results (fig. 4.6a) resemble the measured place cells in rats (fig. 4.6b).
4.2. APPLICATIONS

Another approach to a similar problem, that aimed to understand the diversification in the visual system, has been made by Wyss et al. They designed an online algorithm based on equation \[1.5\] with a nonlinear function class.

As for Franzius et al., the key element was a hierarchical processing of overlapping receptive fields with the same learning principle in every layer. The video images were of smaller resolution and they used 5 instead of 3 layers. The main differences resides in the use of a real robot and another magnitude of training examples: 66h at 25 Hz \(\approx 6 \cdot 10^6\) frames \[11\] in comparison to "a few laps within 5,000 samples" \[42\].

The results of the last layer are orientation invariant and look like (big) place cells (fig. 4.5), but since no theoretical solutions are available, it is hard to comprehend why. In the end the results of Wyss et al. set up more questions than they answer, so this thesis sticks with the methodology of Franzius et al.

Figure 4.4: SFA responses from Franzius et al. [42]. Every pixel in a sub-image represent one position in a square room. The colors indicate SFA responses. Image source: Poster presentation by M. Franzius at the 2007 meeting of the German neuro-science society.

Figure 4.5: Two examples for every layer of Wyss et al. [41]. The left of each example is the mean response at every position and the right represents the orientation stability in all directions within one standard deviation (gray).
4.3 Algorithms

In this thesis we want to use optimization problem 4.1 i.e. the formalism developed by Wiskott et al. First we will review linear SFA and its common extension, to finally define a kernelized SFA algorithm. The latter is novel in this form, but has similarities to existing works.

4.3.1 Linear SFA

We aim to find a set of $k$ functions that solve minimization problem 4.1 with respect to $n$ observations $\{x^{(i)}\}_{i=1}^{n} \subset \mathbb{R}^d$. Despite the name, we consider affine functions $\phi_i(x) = w_i^\top x - c_i$ as model class. To keep the notation simple, we use a matrix notation of filter responses ($\Phi$ and $\dot{\Phi}$, as defined before) and observations $X_t = x^{(t)}_i$ and $\dot{X}_t = x^{(t+1)}_i - x^{(t)}_i$.

The $k$ solutions are calculated simultaneously in 3 steps:

1. **Centering of the data**: $x_c = x - \bar{x}$, where $\bar{x} = \mathbb{E}[x]$.

2. **Sphering of the centered data**: $x_s = S x_c$, where $\mathbb{E}[x_c x_c^\top] = \mathbf{I}$. Sphering establishes unit variance and decorrelation. An eigenvalue decomposition of the covariance matrix $\mathbb{E}[x_c x_c^\top] = \frac{1}{n} X X^\top - \bar{x} \bar{x}^\top = U \Lambda U^\top$, can be used to determine the sphering matrix $S = \Lambda^{-1/2} U^\top$.

3. **Minimizing the slowness**: This can only be achieved by a rotation of the sphered data, since any other operation would violate the already fulfilled constraints. Again, an eigenvalue decomposition of a covariance matrix
4.3. ALGORITHMS

Algorithm 9 Linear SFA

Require: $k \in \mathbb{N}^+$; $\{x^{(i)}\}_{i=1}^n \subset \mathbb{R}^d$

// Collect covariance matrices
$\bar{x}_1 = x^{(1)}$
$C_1 = x^{(1)}x^{(1)\top}$
$\hat{C}_1 = \text{zeros}(d,d)$
for $i = \{2,\ldots, n\}$ do
  $\dot{x}^{(i)} = x^{(i)} - x^{(i-1)}$
  $\bar{x}_i = \bar{x}_{i-1} + \dot{x}^{(i)}$
  $C_i = C_{i-1} + x^{(i)}x^{(i)\top}$
  $\hat{C}_i = \hat{C}_{i-1} + \dot{x}^{(i)}\dot{x}^{(i)\top}$
end for

// Calculate sphering matrix $S$
$U\Lambda U^\top = \text{eig}\left(\frac{1}{n}C_n - \frac{1}{n}x_nx_n^\top\right)$
$(\hat{U}, \hat{\Lambda}) = \text{remove_zero_eigenvalues}(U, \Lambda)$
$S = \hat{\Lambda}^{-1/2}\hat{U}^\top$

// Find $k$ slowest direction in sphered data
$U\Lambda U^\top = \text{eig}\left(\frac{1}{n-1}SC_nS^\top\right)$
$(\tilde{U}_k, \tilde{\Lambda}_k) = \text{remove_all_but_lowest_k_eigenvalues}(\hat{U}, \hat{\Lambda}, k)$

// Return affine function $\phi(x) = W^\top x - c$
$W = S^\top \tilde{U}_k$
$c = \frac{1}{n}W^\top \bar{x}_n$
return $(W, c)$

$\mathbb{E}[\dot{x}_i \dot{x}_i^\top] = \frac{1}{m-1}S\dot{X}\dot{X}^\top S^\top = \tilde{U}\tilde{\Lambda}\tilde{U}^\top$ can be used. The solutions are given by the eigenvectors $\tilde{U}_k$ corresponding to the $k$ smallest eigenvalues.

Combining the steps, the affine function $\phi$ is given by $\phi(x) = W^\top x - c$, where $W = UA^{-1/2}\tilde{U}_k$ and $c = W^\top \bar{x}$. Since the eigenvalue decompositions have complexity $O(d^3)$, algorithm 9 has an overall complexity of $\max(O(d^n),O(d^3))$.

4.3.2 Expanded SFA

When linear SFA does not yield sufficient slowness, i.e. linear functions are too weak, we might wish to use a nonlinear function class. A common way is to expand the data into a nonlinear feature space and perform linear SFA on the expanded data [35].

The most popular expansion is the set of all monomials up to degree 2 (quadratic expansion) [38, 42] or degree 3 [39]. Linear SFA with these expansions
is sometimes referred to as quadratic SFA and cubic SFA, respectively. Since the dimensionality of expanded inputs grows rapidly, most authors reduced it first with a principal component analysis (PCA) \cite{11}. Because monomials of extreme positions can also take extreme values, Franzius et al. included a clipping of high outputs in their procedure \cite{42}.

### 4.3.3 Kernel SFA

The idea of projection into a high dimensional feature space reminds of kernel techniques, so we might avoid explicit expansions and develop a kernelized SFA algorithm, instead. For a related cost function a kernel approach has already been made by Bray and Matrinez \cite{36}. Besides the difference in the cost function their approach differs from this one because they do not use a kernel matrix but work directly with support vectors. Using the projected process kernel matrix approximation method, their approach turns out to be a special case of this algorithm. In the following let $k(\cdot, \cdot)$ be a given kernel and $\psi(\cdot)$ the corresponding feature mapping. For a definition of these terms, read section 2.2.

Again, we group the data projected in feature space in a matrix $\Psi = \psi_i(x(t))$.

1. **Centering** can be performed directly on the kernel matrix (sec. 2.2.4): $K_c = (I - \frac{1}{n}11^\top)K(I - \frac{1}{n}11^\top)$. Note that we implicitly centered the data in feature space this way, since $K_c = \Psi_c^\top \Psi_c$.

2. **Sphering**: As discussed in section 2.2.4, we substitute the nonsingular eigenvectors $U$ in the sphering matrix (in feature space) with those of the kernel matrix: $S = \frac{1}{\sqrt{n}}\Lambda^{-1}_r V_r \Psi^\top$.

3. **Minimizing the slowness**: Let $\hat{\Phi} := \Phi D$, with $D \in \mathbb{R}^{n \times n-1}$ being a matrix which is zero everywhere except for $D_{1,i} = -1$ and $D_{i+1,i} = 1$. This way we can express the covariance matrix $\frac{1}{n(n-1)}A^{-1}_r V_r \hat{\Phi} \hat{\Phi}^\top S^\top$ in feature space as $\frac{1}{n(n-1)}A^{-1}_r V_r \hat{\Phi} \hat{\Phi}^\top S^\top$ with $\hat{K} = \Psi^\top \Psi D$. The eigenvectors corresponding to the smallest $k$ eigenvalues of this covariance matrix are the rotations $\hat{U}_k$ which optimize the problem.

The kernel solution to optimization problem \cite{11} is given by $\phi(x) = A^\top k(x) - c$, with the weight matrix $A = (I - \frac{1}{n}11^\top) V_r \Lambda_r^{-1} U_k^\top$, the kernel expansion $k(x) := [k(x^{(1)}, x), \ldots, k(x^{(n)}, x)]^\top$ and the bias $c = \frac{1}{n}A^\top K1$.

The algorithm collects the matrix $K$ and derives $\hat{K} \hat{K}^\top$ from it. The two eigenvalue decompositions in steps 2 and 3 are responsible for an overall complexity of $O(n^3)$.
Algorithm 10 Kernel SFA with kernel matrix approximation

Require: $\hat{k} : \mathbb{R}^d \times \mathcal{P}(\mathbb{R}^d) \rightarrow \mathbb{R}^m$; $k \in \mathbb{N}^+$; $\{\hat{x}^{(i)}\}_{i=1}^m \subset \{x^{(i)}\}_{i=1}^n \subset \mathbb{R}^d$

// Collect kernel matrices
// In the following: $\hat{k}^{(i)} := \hat{k}(x^{(i)}, \{\hat{x}^{(i)}\}_{i=1}^m)
\hat{k}_1 = \hat{k}^{(1)}$
$\hat{K}_{1}^\top = \hat{k}^{(1)} \hat{k}^{(1)} \top$
$\hat{K}_{1}^\top = \text{zeros}(m, m)$
for $i = \{2, \ldots, n\}$ do
$\hat{k}_i = \hat{k}^{(i)} - \hat{k}^{(i-1)}$
$\hat{K}_i^\top = \hat{K}_{i-1}^\top + \hat{k}^{(i)} \hat{k}^{(i)} \top$
$\hat{K}_i^\top = \hat{K}_{i-1}^\top + \hat{k}^{(i)} \hat{k}^{(i)} \top$
end for

// Calculate sphering matrix $S$
$S = \Lambda^{-1/2}_r U_r^\top$

// Find $k$ slowest direction in sphered data
$U_k \Lambda_k U_k^\top = \text{eig}(\frac{1}{n-1} \hat{K}_n^\top \hat{K}_n S)$
$(U_k, \Lambda_k) = \text{remove}_\text{all but lowest}_k \text{eigenvalues}(U_k, \Lambda_k)$

// Return kernelized function $\phi(x) = A^\top \hat{k}(x, \{\hat{x}^{(i)}\}_{i=1}^m) - c$
$A = S^\top U_k$
$c = \frac{1}{n} A^\top \hat{k}_n$
return $(A, c)$

Kernel matrix approximation Kernel SFA performs much better than linear SFA, but raises the complexity to $O(n^3)$. One would like to apply the projected process method described in section 2.2.6, but this method only provides approximations of $K^2$. As already discussed, $K^2 = V \Lambda^2 V^\top$ has the same eigenvectors and squared eigenvalues of $K$. If we perform the eigenvalue decomposition on $K K^\top$ and take the square-root of the eigenvalues, the solution is the projected process approximation of $K$.

With this approximation, algorithm 10 has complexity $O(m^2 n)$ because it requires the collection of the matrices $\hat{K} K^\top$ and $\hat{K} K^\top$. Additionally, one has to pick a set of support vectors, which usually is costly, too. For more information on the selection of support vectors, read section 2.2.6.
4.4 Conclusion

Slow feature analysis is a unsupervised method to extract the current state out of any data with a temporal structure. It learns an array of filters that aim to extract all non-static parameters that distinguish the input from other samples. Given a powerful function class and enough training samples, the output will converge to a trigonometric representation of the current state, as far as it can be extracted out of the current input. As such it is well suited for the approximation of continuous functions on this state, as the discussion of trigonometric representations in section 3.1.3 shows.

However, instead of converging to the theoretical optimal responses, filters with equal slowness can mix linearly. This is not a problem for function approximation, since the mixed solutions span the same space of trigonometric basis functions. If, on the other hand, one is only interested in a subset of the state components, e.g. only the spatial component of the state space described in proposition 4.4, the mixture prevents simple exclusion of unwanted filters. Because the number of filters grows exponentially in the number of state components, every unwanted component is a nuisance. If possible, one can obtain at least the first few filters undisturbed by controlling the relative velocity between state components in the training set.

Under controlled circumstances (e.g. in a simulator) we are interested in the whole state space and can therefore ignore these effects. Real life experiments, however, have shown many additional components, e.g. altitude of the sun, artificial light, etc. Every independent source of change in the light conditions is considered a state component as well as any change in the actual scene.

At last one has to point out that this method can only be applied to static scenes. Something as complex as a group of humans induces a state space far too complex for any function class feasible in the near future.
Chapter 5

Empirical validation

5.1 Experiment description

The main experiment of this thesis is a proof of concept of the following proposition:

Proposition 5.1 Policy iteration can learn a control based only on a current video image, which is preprocessed with filters obtained by slow feature analysis.

We showed in chapter 4 that SFA, applied on a random walk in bounded state spaces, converges to filters that form a trigonometric representation of this state space. This claim holds, independent of the representation in which the state is originally presented to SFA. Therefore, the state can be presented in form of video images, recorded from the perspective of a robot which is moving through a static scene. SFA will converge to a trigonometric representation of the robot's position.

As we have shown in chapter 3, the policy iteration method LSPI is able to learn a control out of a random walk presented in any representation. Of course, the quality of the control depends on representation and considered function class. However, we have also shown that trigonometric representations are especially suited for the class of linear functions, as employed by LSPI.

To validate this approach, we chose a navigational experiment in which a robot is supposed to drive into a goal area. The only available sensor is a head mounted camera. Obviously, its video images are too high dimensional\footnote{LSPI has a complexity of $O(a^2d^2)$ in space and $O(a^3d^3)$ in time, where $a$ is the number of actions and $d$ the dimensionality of the state representation.} and too complex\footnote{For example, a small rotation of the robot leads to drastic changes in nearly every pixel.} to promise LSPI solutions with reasonable quality.

However, as results in section 5.3.3 show, after preprocessing the learned control was able to find the goal in $\approx 80\%$ of the test trials.
Figure 5.1: The experiment: a) Record a random walk video with the robot. b) Learn the SFA filters based on this video. c) Estimate the Q-value based on the preprocessed video. d) Validate the control at random start positions.

5.1.1 Overview
The main experiment is conducted in 4 phases, as depicted in figure 5.1:

a) Record of a random walk video with a camera mounted on the head of a robot.

b) Learn a preprocessing based on the random walk video with kernel SFA.

c) Estimate the Q-values based on the preprocessed random walk video with LSPI, to derive a near optimal policy.

d) Validate the learned control at random positions by choosing the action associated with the highest Q-value until the robot reaches the goal.

5.1.2 Formal description
Task The task is to navigate as quick as possible into a goal area. This area is not marked or discriminable to other parts of the environment, besides by the reward given when the robot is inside. The only other reward is a punishment for getting too close to walls, i.e. most of the environment is without reinforcement signal.

Environment The environment is static, bounded and the robots position recognizable almost anywhere based on the camera images. That means we have a closed room which is asymmetric at least in the textures and therefore has few positions that resemble each other, which is the case in many indoor scenarios. It is the claim of staticity that introduces the most problems, since it restricts the application to uninhabited areas. It is, however, a restriction of the slow feature analysis and therefore necessary for this thesis.

Behaviour We assume decisions at discrete time steps between a limited number of discrete actions. As a side effect, the discretization liberates us of any time constraint. The learning algorithm does not know the actions in use, but they have to allow the robot to navigate anywhere. For our experiments we chose 3 actions: move forward ca. 30cm and turn left/right ca. 45 degrees.
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Figure 5.2: The wheeled Pioneer 3DX robot used in the experiments, a picture from the head mounted camera and from the observing camera at the ceiling.

5.1.3 Robot

For simplicity, the robot is assumed to be wheeled and is able to execute commands like "turn 45 degrees" or "move 30cm". However, the execution can be flawed, e.g. the robot can turn 48 degrees instead of 45 or move 32cm instead of 30. The NeuRoBot project used the Pioneer 3DX robot build by Mobilerobots Inc (fig. 5.2a).

Camera The head mounted camera has a wide field of view to impede similar images at different positions. Beside this, the only restrictions are a reasonable resolution and image quality. The Bumblebee® camera used by NeuRoBot has a field of view of 66°, which seems to be sufficient anywhere but directly in front of walls. It also records a pair of stereo images, of which we only considered the left one (fig 5.2b).

Other sensors For navigation, no other sensors are necessary. The considered policy iteration method, however, requires a random walk before training. This implies at least one dependable sensor system to avoid/react to walls during this phase. The Pioneer 3DX is equipped with ultrasonic sensors and sensitive bumpers. To treat the test environment with care, we employed the ultrasonic sensors to avoid walls during random walk.

Validation To validate the learned control, one needs to know the robots position in training and testing. The internal position estimator of the Pioneer 3DX turned out to be useless, since local estimation errors are integrated over time. After a few minutes, the error was unacceptable. Instead, we installed a web cam at the ceiling and extracted the position of the illuminated blue and red ball on the robots head from it (blue and red squares in fig 5.2c).
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Figure 5.3: Illumination changes drastic under daytime conditions.

5.1.4 Environment

In more detail, the requirements on the environment are:

- **Bounded space**: Training SFA requires to travel the whole state space, multiple times if possible. An open field (without boundaries) would make this impossible, therefore we need a closed room.

- **Asymmetry**: If two positions produce the same image, SFA will assign both positions the same response. This violates the assumption that the learned representation of states is injective (def. 3.7).

- **Static scene**: The robots position is the only variable in the environment. If other factors change the image reliably, e.g. whether an operator is in the room or not, they will introduce new SFA filters. This would increase the number of extracted filters without gaining additional information useful for the navigation problem.

As it turns out, natural light conditions are not static at all. The sun’s position and every cloud shifting in front of it changes illumination and reflection in the scene. Due to the build-in brightness correction of the camera, the images suffered shifts in color, contrast and brightness almost independent of the robots position (fig. 5.3). To circumvent this, we restricted our experiments to artificial illumination at night. Reflection and brightness still change, but remain almost static with respect to the robots position.

The experimental environment used in this thesis consists of a rectangular $3m \times 1.8m$ area, which is bounded by tilted tables and a wall. All four sides were covered by the randomly assembled wallpaper in figure 5.4. The walls were ca. 90cm in height, so the robot could see parts of the laboratory and therefore the human operators. To avoid human interference, the upper part of the image was clipped out (as depicted in fig. 5.8).

Figure 5.4: Randomly assembled wallpaper of the experimental environment.
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5.1.5 Simulator

Working with the PIONEER robot, however, proved to be time consuming. In addition, producing high resolution test maps (sec. 5.1.6) is nearly impossible.

The author implemented a simulated version of the experiment to verify the results in large scale tests. The simulator is written in Java3D and communicates with the MATLAB implementation of algorithm 8 by providing a network service. The render engine does not provide shadows or directed illumination (only ambient light). Instead it relies on photographed textures of walls and laboratory.

Figure 5.5 shows an overview of the rendered environment from a ceiling camera perspective. It also gives three example images and their real-life counterparts, recorded by the robot. The first difference one will notice is the difference in color. The textures were photographed at daytime, the camera images
recorded at night. Artificial light has a shift to yellow compared to sun light reflected on white walls. The second inaccuracy is the unrealistic floor texture. The whole floor as texture simply did not fit into the graphic cards memory. Additionally, the real floor provides reflections that could not be modelled properly. At last, the BUMBLEBEE camera lens distorts the outer areas of the image, which also could not be simulated.

The simulator is not meant to copy reality perfectly, but to allow a thorough verification under similar conditions.

Other environments Until now we remained inside the boundaries of theory. We know that slow feature analysis converges to a trigonometric representation in rectangular rooms. The only remaining question is how well (which will be answered in section 5.2). Predictions for other room geometries, however, are hard (and maybe impossible) to derive, so the question arises how SFA will handle such a case. With the simulator at hand, we will examine this question for an example room.

Many room shapes are possible and interesting. We chose two quadratic rooms, connected by a small corridor, which we will call two-room environment (fig. 5.6). Since we do not have to rebuild any existing room, we are free to use publicly accessible libraries of textures, from which we chose an Egyptian theme. To make the scene more appealing the author decided to place one room outdoors, restricted by a wall of medium height. To prevent similar images at different positions, all "inside" walls differ in portrayed reliefs and "outside" a couple of different sized pyramids were placed arbitrary in the far distance.

5.1.6 Video generation

Both policy iteration and slow feature analysis need random walks as training sets. Both methods require balanced sampling over the whole state space.

As simple as a random walk is to implement, the robot can get caught between boundaries as trivial as rectangular corners. Special movement statistics (as required for place cells, sec. 4.2.3) and coarse actions (as the proposed 45° rotation) introduce additional jamming opportunities. Instead of facing these difficulties we decided to record one video (in three sessions) with movement statistics that seem to visit all parts of the environment equally often. Out
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of this video we sampled one training set for SFA and one for policy iteration. Since we recorded the random walk with the ceiling camera, we were able to duplicate it in the simulator.

The more complex the environments geometry gets, the more likely is a random walk to get stuck. For example, in the two room environment the connecting corridor is a bottleneck. It is much more likely to stay in the room than to hit the corridor and change it. In the long run this effect will cancel out statistically, but with limited training samples it is unlikely to obtain a balanced set by random walk.

Since we only performed this experiment with the simulator, we sampled the training set as pairs of successive frames at random start positions and movements. This may sound unrealistic but is an easy way to achieve guaranteed uniform distributed training samples.

**Test sets**  Sampling a test set (unseen in training) out of the random walk is not complicated. However, sampling a *meaningful* test set is.

To compare the orientation/place independence of single filters one optimally expects a high resolution training set of images at equidistant coordinates with the same orientation. A set of these *test maps* with different orientations, can give an overview of the filter responses.

The simulator can produce exact test images, so we created a set of 8 test maps (in 45° steps) with 64 × 32 equidistant coordinates, each (e.g. in figure 5.11b). Creating test maps for the real experiment, however, is not that trivial.

To find a test set which comes near to the described test map, we filtered all frames within 5° of the desired target map orientation. Out of this set, we used frames as equidistant distributed as possible. As a result, we can only give a scatter plot of the test map in which the test samples can differ in angle up to 10° (e.g. in figure 5.11).

**Image resolution**  Kernel SFA with projected process matrix approximation (algorithm 10) has a complexity of $O(m^2)$ in space and $O(m^2n)$ in time. Here $m$ is the number of support vectors and $n$ the number of training samples. This complexity does not seem to be affected by the input images dimensionality $d$.

However, We have to store the support vectors and perform a kernel expansion at every frame, too. This induces an additional complexity of $O(md)$ in space and $O(mdn)$ in time (assuming a kernel with complexity $O(d)$ in time,
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Figure 5.8: Video image preparation steps.

e.g. the RBF kernel). As long as \( d < m \), this cost does not exceed the cost of performing kernel SFA and we are relatively free to choose the image resolution. If we exceed this threshold significantly, however, the new costs depend linear on the number of pixels, which is quadratic in image resolution. For example a \( 320 \times 240 \) RGB image contains \( d = 230400 \) independent values which exceeds the maximum number of support vectors used in this thesis \( (m < 8000) \) by a factor of 28. Therefore, we scaled the image down to a relatively conservative resolution of \( 32 \times 16 \) RGB pixels \( (d = 1536) \). To investigate the influence of image resolution, we also duplicated one experiment with a resolution twice as high \( (64 \times 32 \) RGB pixels \( \Rightarrow d = 6144 \), see section 5.2).

Keeping considerations from section 5.1.4 in mind, we performed a three step transformation on the original video images before presenting them to SFA (see fig. 5.8 for the process and fig. 5.7 for the results):

1. Clip out the upper 80 lines to avoid human interference from the laboratory.
2. Correct mean brightness to counter the cameras automatic adjustment.
3. Shrink the image to size \( 32 \times 16 \).

5.1.7 Alternative approaches

Most reinforcement learning approaches have customized representations (see for example Stone and Sutton [25]). These are not comparable to an adaptive technique like SFA. To the authors knowledge, no other approach can estimate the current position based on a single frame.

The technique coming closest to position estimation based on video images is called simultaneous localization and mapping (SLAM or Visual SLAM in the context of video input). Originally, Smith et al. [45] investigated the problem for vehicles with sonar sensors. Roughly a decade ago, Davison [46] adapted the method to Visual SLAM, which is currently under development by several groups [47, 52, 53].
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The classical solution, as well as many modern approaches [40, 53] employ extended kalman filters (EKF) to estimate landmark positions. These suffer \(O(n^2)\) complexity in the number of landmarks \(n\), due to statistic dependencies between their estimation. Landmarks are small 2d patches with their estimated 3d position, which should be as relocatable as possible. For this, a variety of 2d transforms are in use, e.g. affine transformation [53] or SIFT [52]. Comparing all possible patches with all known landmarks is computationally expensive [52]. Instead, it is possible to incorporate information about the expected location in so called active measurement strategies. This way, Visual SLAM can be performed in real time [47, 49, 53].

To cover larger environments, the Rao-Blackwellized particle filter was first introduced by Murphy [50] followed by a practical framework by Montemerlo [51]. Out of the perspective of every particle, the camera position is fixed and the landmark estimation thus independent, yielding \(O(mn)\) complexity for \(m\) particles. In the field of Visual SLAM, Sim et al. [52] and Eade et al. [53] successful applied these particle filters.

Alternatively, Estrada et al. [48] extended the EKF approach by producing independent local maps of limited size. These are stitched together in a global layer thus the algorithm is called hierarchical maps. Recently, Clemente et al. [49] applied this approach to Visual SLAM.

Whereas Visual SLAM is a well established field with remarkable success, our approach differs in some mentionable ways:

- SLAM depends on a specific type of sensor input, whereas SFA automatically adapts to any sensor.
- SLAM holds a current state, which is crucial for localization and prone to initialization errors. In contrast, SFA works instantaneous and can localize the robot using one frame only.
- SFA extracts a trigonometric representation of the position. SLAM, on the other hand, estimates position in 3d coordinates.

To compare SFA to SLAM, one would have to expand the position estimates to a trigonometric representation. These could be used instead of the SFA output to learn a control. Because SLAM algorithms are quite complex and not easy to use, the author could not provide such a comparison in the available time.

Anyway, even if we could, SLAM is bound to have an internal state. Comparison would only be fair when we grant such a state to SFA, too. This would violate the proof of concept approach of this thesis.
5.2 Learn preprocessing

Before we learn the navigational control in the next section, we want to validate the theoretical predictions of SFA as a preprocessing (chapter 4). The main concern is, how well kernel SFA performs in our context, i.e. how close to the optimal responses one can come with current computers.

We evaluate different SFA algorithms, which in fact reflect different function classes fitted to optimize the SFA cost function (sec. 4.1.1). The point of reference are always the optimal responses that can be expect in the limit (sec. 4.1.2).

The videos We recorded 3 videos in different environments to test SFA predictions (sec. 5.1.4, 5.1.5 & 5.1.6):

- **Robot experiment**: The original random walk video recorded by the Pioneer robot. We reduced the frame rate to \( \sim 1 \text{Hz} \), resulting in 35128 frames under relative stable conditions at night.
- **Simulated experiment**: Due to the ceiling camera, we were able to record the same trajectory as in the robot experiment in the simulator.
- **Two room experiment**: To test the SFA responses in different geometries, we recorded a simulated training set in the two room environment. The video contains 35000 random transitions at random start positions.

The algorithms We applied linear SFA (algorithm 9) directly on the raw video images. This algorithm restricts the image resolution stronger than kernel SFA. Using \( 32 \times 16 \) RGB pixel images turned out to be feasible without problem, but \( 64 \times 32 \) RGB pixel images rise the computational demand by a factor of 64. We therefore had to omit the latter experiment with linear SFA.

Our main focus centered on kernel SFA (algorithm 10). Because all videos contain \( \sim 35000 \) frames, we employed the projected process kernel matrix approximation method with a greedy support vector selection (algorithm 4). Through the number of support vectors, one indirectly controls the model complexity of this approach. Therefore it is especially suited to investigate the SFA behaviour for different function classes. While the complexity of kernel SFA is susceptible to large image resolutions too, the \( 64 \times 32 \) pixel resolution did not cause overwhelming overhead, as for linear SFA.

We only considered the RBF kernel (sec. 2.2.3). Other kernels seemed promising too, but RBF kernels proved to be very reliable as long as the support vectors are drawn out of the complete state space. Because the greedy selection algorithm allows only a hyper parameter \( \nu \) to adjust the sparsity of the support vector set (sec. 2.2.6), finding a suitable sized set demands multiple trials with either changed \( \nu \) or kernel parameter \( \sigma \). Because we have no other means to determine a good \( \sigma \), we decided to vary it and keep the sparsity parameter fixed at \( \nu = 0.1 \).
Figure 5.9: Mean slowness on the training set of the robot experiment for different SFA classes and kernel matrix approximations as number of support vectors (SV). 32 × 16 and 64 × 32 denote the image resolution. Note that linear SFA does not use support vectors and the theoretical solutions are the slowest functions possible.

5.2.1 Slowness

The foremost question is whether the considered SFA algorithms are able to produce a trigonometric representation of the robot’s position. Since SFA filters are likely to be mixtures of optimal responses, a direct comparison is only possible in the slowest, unmixed filters.

Instead, one can compare the slowness of SFA filters and optimal responses on the training set. We know that no filter can be slower than the optimal responses, so the difference in slowness can serve as a measure how well SFA has converged to a trigonometric representation. Because this does not involve any test sets, we compared the slowness in the robot experiment, as it is the most realistic case.

In figure 5.10, the slowness of all filters obtained by kernel SFA with different sets of support vectors are plotted. One can observe that the first filters are much closer to the optimum than latter ones, which are more likely to be influenced by (fast) noise.

Figure 5.10: Slowness of all SFA filters in the robot experiment for different number of support vectors used by kernel SFA. Note how close the slowest filters of the 7704 SV line are to the optimum.
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Figure 5.11: Comparison of the first 6 filters of (a) the robot experiment with 7973 SV and (b) the simulated experiment with 8064 SV.

To see how close the results are to a trigonometric representation, figure 5.9 plots the mean slowness every 10 filters against the number of support vectors used. Note that linear SFA is comparable to kernel SFA with \( \sim 700 \) SV and that the slowness seems to converge against the optimum with more SV.

Another noteworthy result depicted in figure 5.9 is that a higher image resolution (64 \( \times \) 32) performs worse at equal model complexity. Given that a higher resolution represents a more complicated problem, it makes sense that easier problems perform better. It can be expected that this relationship will switch at a high model complexity, since the high resolution images contain more information. Due to current computational limitations, we were not able to verify this prediction.

5.2.2 Responses

Having established the performance of kernel SFA in terms of slowness on the training set, we now want to verify the predictions on test sets. Because of the inherent inaccuracy of the robot experiment test set, we will focus mainly on the simulators results.

Figure 5.11 shows test maps of the first 6 filters of both experiments in two opposite directions. While the first filter looks more or less the same, the

![Figure 5.12: SFA filter \( F_1 \) of the simulated experiment resembles optimal response \( \phi_{100} \).](image)

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5.2. LEARN PREPROCESSING

Figure 5.13: SFA filters 2 and 3 of the simulated experiment with 8064 SV resemble mixtures of optimal responses $\phi_{200}$ and $\phi_{001}$, as predicted in proposition 4.5.

later ones differ significantly. Since the trajectory (and therefore the movement statistics) are the same, the only explanation is the difference in images, which led to another solution.

We can also observe that the first filter in both experiments look like the optimal response $\phi_{100}$, which is depicted in more detail in figure 5.12. In the robot experiment, the second filter also resembles $\phi_{200}$. In contrast, the second simulator filter is not even orientation invariant. The latter situation is shown in figure 5.13. As theoretical predicted in proposition 4.5, SFA filters with the same slowness can mix, e.g. $F_2 \approx a\phi_{200} + b\phi_{001}$ and $F_3 \approx b\phi_{200} - a\phi_{001}$ as long as $a^2 + b^2 = 1$. We see here a mixture of the second orientation invariant basis function in horizontal direction $\phi_{200}$ (filter 2 in the robot experiment) with the first place invariant basis function $\phi_{001}$.

Filters above 3 are hardly similar to any optimal response, but as filter 2 and 3 showed, they might as well be arbitrary rotations in the subspace of basis function with equal slowness.

5.2.3 Other environments

As close as the previous results came to the predicted responses, it is of great practical interest how far they will differ when we leave the domain of theoretically predictable environments. The responses of the two-room experiment should give us some insight at a simple yet common example.

Figure 5.14 shows the response of first 6 filters from a birds perspective. In difference to the rectangular room, the filters seem to specialize in single rooms. Interestingly, in the chosen room the response look like a trigonometric basis function. For example, the filters 2 and 6 resemble the optimal response $\phi_{100}$ in one room, but are near zero (green color) in the other. In this sense, filters 3 and 5 resemble optimal response $\phi_{010}$. Higher filters are less intuitive, since as before they mix strongly with orientation sensitive responses of equal slowness. However, in the limit, one would expect two full sets of trigonometric basis functions, that each span one room exclusively.
As promising as these results look in terms of function approximation, unexpected filters also emerge. For example, filter 1 resembles a room ID function which is positive (red) in the left and negative (blue) in the right room. While this somehow still fits in the room specific framework described above, filter 4 seems to be active in the center of both rooms.

5.2.4 Discussion

We were able to verify that, with growing sets of support vectors, kernel SFA filters converge to trigonometric basis functions of the robots position. At some examples, we could also find evidence for other theoretical predictions, like mixture of basis functions with equal slowness. Leaving the area of predicted room shapes, the results also look promising, albeit not all filters resemble trigonometric basis functions.

In conclusion, SFA indicates to be a well suited preprocessing for linear value approximation. The inherent property of mixtures in basis functions, on the other hand, forces us to extract the complete state space. These mixtures seem to follow a broad interpretation of "equal slowness", i.e. all features but the first few mix with at least one other. Without any means to un-mix the basis functions, we can not exclude unwanted states (like humans, sun position or blinking lights), and are therefore restricted to static scenes.

The adaption to a two room environment apparently led to a functional basis for each room, and some unique additional filters. A partition in separate rooms can actually be seen as an advantage. For example, it reduces the number of involved filters when the behaviour is learned in one room only. This could be exploited by a clever reinforcement algorithm to reduce the computation time.

Some filters do not fit in this scheme and seem to be useless in terms of function approximation. However, without analytical solution it is hard to validate such statements.
5.3 Learn navigation

First, we want to validate the performance of policy iteration with a trigonometric representation (sec. 5.3.2). To compare policies, we also define a quality measure named convergence quality and show how well the learned control behaves compared to a near optimal hand-crafted reference policy.

In section 5.3.3, we will learn navigational control based on video images only. Here we validate the advantage an SFA preprocessing yields and how alternative room geometries influence the performance.

The algorithms

Given a training set in any linear representation (def. 3.7), we use LSPI (algorithm 7) to learn the optimal policy. LSPI employs LSQ (algorithm 6), which in turn calls LSTD (algorithm 5), to estimate Q-values. We chose a discount factor of $\gamma = 0.9$ in the laboratory and $\gamma = 0.95$ in the two room environment because the latter was of much bigger size.

After determining the best policy, the control (algorithm 8) navigates by letting the policy choose one of the 3 actions: move forward ca. 30cm, rotate left 45° or rotate right 45°.

The representation, the reward distribution, and the training set influence the resulting policy.

Robot training set

We were able to extract a set of 3091 rotations and 5474 movements out of the random walk video recorded by the robot. After mirroring the rotations (if $x_2$ is 45° to the right from $x_1$, then $x_1$ is 45° to the left of $x_2$), we reached a training set of 11656 transitions.

A reward of +1 was given for entering the goal area, and a punishment of -1 for coming too close to the walls (< 50cm). We tested two goals, the center of the room with a radius of 20cm (fig. 5.15a) and the lower right corner with a radius of 45cm (fig. 5.15b).

![Figure 5.15: The test set (dots) for the robot- and simulation-experiment, colored in received reward (blue: -1, green: 0, red: +1), for two different goals.](image-url)
CHAPTER 5. EMPIRICAL VALIDATION

Figure 5.16: The test set (dots) for the two-room experiment, colored in received reward (blue: -1, green: 0, red: +1).

Two room training set  As discussed in section 5.1.6, we sampled the random transitions uniformly. Because the environment is larger, we decided to use a training set of 50,000 transitions. Figure 5.16 shows the distribution and received reward of the used training set.

It took the author some time to find a working reward distribution. There are many hyper parameters to set and some were surprisingly influential. Two observations stroke us as particular noteworthy:

(1) The discount factor $\gamma$ has an undeniable impact on the learned control. Large environments seem to require large $\gamma$. One explanation would be the exponential decay of value the more one departs from the goal area. The quadratic cost function of LSTD distributes the approximation error equally on all samples. As a result, areas of close-by Q-values will be more likely to pick the wrong action. This includes all areas far away from the goal where the overall value is small. Therefore, large environments need to ”spread” the positive reward further, i.e. need a larger $\gamma$, to counter this effect.

(2) When the punished distance to walls is too large, the positive reward is not propagated in the other room. Most likely, the close proximity to negative reward prevented the distant positive reward to be propagated through the corridor. However, since this is no theoretical handicap, it must be a result of weak approximation at this critical point.

5.3.1 Policy evaluation

Evaluating a learned policy is more complicated than in the case of, for example, regression. Applying the policy on a representative test set (e.g. a test map as described in section 5.1.6) shows us the distribution of actions, but does not allow any conclusions about the controls behaviour. For example, there could exist ”loops” from which the robot can not escape and never reach the goal. Therefore we have to evaluate the trajectories, produced by the policy.

The initial task of this experiment was to reach the goal area as quickly as possible. Counting the steps to the goal $\tau(\pi, x_0)$ would be the most intuitive
measure how well a policy $\pi$ fulfills this task at some start position $x_0$. However, since we are interested in the quality of all possible trajectories, an area of "loops" (i.e. that can not be left) would drive this measure to infinity.

The approach we want to take here uses the value $V^\pi(x_0)$ to evaluate the policies fitness. Given the simplified case that we ignore punishment at walls and treat the goal area as absorbing states, this measure is a modification of the former: $V^\pi(x_0) = \gamma^{\tau(\pi,x_0)} - 1$. On the one hand, this measure can handle infinitely long trajectories. On the other hand, compared to the optimal policy $\pi^*$, unnecessary detours near the goal have more influence on the measure that those far away. When this is not desired, one can normalize the result with the optimal value $V^{\pi^*}(x_0)$. We will call the mean of this ratio the convergence quality:

**Definition 5.1 (Convergence quality)** Let $p(x)$ be a uniform distribution over the state space of $x$, except the goal area, and let $V^\pi(x)$ denote the value of state $x$, with a reward of 1 at the absorbing states of the goal area. Given the optimal policy $\pi^*$, the following will be called convergence quality:

$$C(\pi) = \int \frac{V^\pi(x_0)}{V^{\pi^*}(x_0)} p(x_0) \, dx_0$$

(5.1)

This measure of policy convergence has some nice properties:

- $C(\pi) \in [0, 1]$ where 1 indicates that $\pi = \pi^*$ and 0 that no trajectories hit the goal.
- $\log_\gamma(C(\pi)) = \int (\tau(\pi,x_0) - \tau(\pi^*,x_0))p(x_0)dx_0$ (mean difference in $\tau(\cdot, \cdot)$ between $\pi$ and $\pi^*$), but does not go against infinity in the presence of loops. The approximation holds only for high $C(\pi)$.

Evaluating the integral in definition 5.1 is not possible but of course can be approximated given example trajectories.

**Reference policy** The definition of convergence quality requires the optimal policy $\pi^*$ that will depend largely on the reward distribution. Building a control that maximizes the sum of expected reward by hand is hardly possible. Instead one can define a policy that aims to reach the goal as quickly as possible. Though this is not $\pi^*$, there is probably little difference in in terms of $\tau(\pi^*, \cdot)$.

Given the coordinates of robot and goal, one can define a simple greedy policy (algorithm 11). The algorithm does not describe the best possible policy, but is probably close to it.

**Two room environment** To use the convergence quality measure in the two-room experiment, one can enhance algorithm 11 by subgoals at each end of the corridor. The new policy would first determine which goal is most reasonable and then call algorithm 11 with the selected (sub)goal.
Algorithm 11 Reference policy

Require: \( p \in \mathbb{R}^2; \theta \in [0, 2\pi] \) // Position \( p \) and orientation \( \theta \) of the robot

Require: \( g \in \mathbb{R}^2 \) // Center of the goal area \( g \)

\[
\Delta \theta = \theta - \text{direction of vector}(g - p)
\]

if \(|\Delta \theta| \leq 45^\circ\) then
    return(MOVE\_FORWARD)
else
    if \(\Delta \theta < 0\) then
        return(TURN\_LEFT)
    else
        return(TURN\_RIGHT)
    end if
end if

5.3.2 Artificial input

Before we apply SFA as a preprocessing, we want to evaluate LSPI on the predicted optimal responses, i.e. trigonometric polynomials. We used the same training set, but instead of the video images we presented the real position in a trigonometric representation. Besides the question how well LSPI will perform, we are also interested in potential overfitting and other factors that would complicate the main experiment.

SFA sorts its filters with respect to slowness on the training set, so we did the same with the optimal responses predicted in proposition 4.4. We omitted mixtures of filters (which appear in SFA, as verified in the last section), because LSTDs result is invariant to rotations of the input space.

Figure 5.17 shows on the left the convergence quality \( C(\pi) \) for the training set (size \( n = 11656 \)) respectively the first half of it \( (n = 5838) \). The goal area resides in the center of the room. The evaluated policies were trained with state representations of a dimensionality \( d \) between 10 and 500, i.e. using the \( d - 1 \) slowest optimal responses and a constant. However, using huge state representations, policies often did not converge at all, so we evaluated every experiment 10 times with different initial policies. The colored areas show one standard deviation and demonstrate how reliable LSPI works.

Though one can observe a regime in which the convergence quality depends largely on the initial policy, it is unclear why. Apparently, some initial actions get in the way of convergence while others lead to good results. This might be due to slight overfitting in the initial value estimation which gets amplified by policy iteration, but there is no analytical explanation that would back up the experimental data.

A simple way to circumvent this problem is to use all possible actions at once, simulating a policy that truly chooses them at random. Superficially, this would triple the training set, but due to the state-action representation in use (def. 3.13) it can be implemented without any computation overhead. The results of this approach are plotted as dashed lines in figure 5.17.
5.3. LEARN NAVIGATION

![Graph showing convergence quality and log convergence quality](image)

Figure 5.17: Left: Convergence quality $C(\pi)$ on artificial state representations for different training set sizes $n$. Every data point on the solid line represents the mean over 10 trials with different initial random policies, evaluated on 1000 trajectories each. The colored area is the respective standard deviation. The dashed line represents a modified initial policy. Right: log $\gamma(C(\pi))$ is an approximation of the mean difference in steps-to-goal between the learned and the reference policy.

no randomness is involved anymore, one experiment per representation size is sufficient.

However, to provide a more intuitive comparison, the right side of figure 5.17 shows log $\gamma(C(\pi))$, which can be considered an approximation for the mean number of additional steps the learned policy needs, compared to the reference policy. Note that the approximation becomes less reliable for low convergence quality values.

In conclusion, one can observe:

1. Using a suitable number of optimal responses (small set/blue area: 20-40, full set/red area: 20-70), LSPI converges reliably to a policy comparable to the reference policy. The mean difference in terms of $\tau(\pi, \cdot)$ in this regime is below one step. We will call this the working regime.

2. More optimal responses (i.e. SFA filters) do not automatically produce better policies. While few input dimensions yield a similar (even though not always good) convergence quality, results of higher dimensionality become unstable. Note that this effect is very similar in both curves, but appears earlier in the smaller training set. This indicates that the effect is the result of overfitting.

3. Sampling all possible actions at once improves the initial policy, doubling the working regime in size. However, since the cause of the unstable regime is unclear, no theoretical statement guarantees an improvement.
5.3.3 Video input

Backed up by the knowledge that LSPI works on the theoretically predicted output of SFA, we proceed with the analysis of LSPI on preprocessed video images.

Simulated experiment First we wanted to know where the working regime with respect the number of used SFA filters is. We therefore repeated the former experiments with the simulated experiment preprocessing described in section 5.2. Utilizing the initial policy modification discussed above, we eliminated the need of multiple trials.

As one can observe in figure 5.18, one needs much more SFA filters to reach a comparable quality. As a side effect, it seems as if we did not reach the overfitting regime, at all. The policies trained with 80 to 500 SFA filters seem to be in the working regime. Though the value is low compared to the predictions, the right side of figure 5.18 shows that this translates only to 2 to 3 steps more than the reference policy.

Figure 5.19: Test trajectories of the robot experiment. The blue triangles mark the start positions and the numbers the length of each trajectory which reached the red goal area.
5.3. LEARN NAVIGATION

Figure 5.20: The same experiments as in figure 5.17, but with \( n = 50000 \) training samples in the \textit{two-room experiment} with artificial state representation.

**Robot experiment** Based on this experiment, we chose \( d = 128 \) SFA filters in the \textit{robot experiment}. A test trajectory driven by a real robot took the author between 5 and 10 minutes and thus generating enough trajectories to estimate the convergence quality was not possible. Figure 5.19 shows all 20 test trajectories and the time each took. With the exception of the lower left area in the right plot the control seems to work reasonably well. However, the steps needed from near by positions vary and most trajectories took surprisingly long.

### 5.3.4 Other environments

Now that we have established our method to be working in simple cases, we want to examine the more complex case of the two-room environment. For once, the length scale is much larger. For example, crossing the environment from left to right, previously done in 9 move-actions, requires 45 actions now. Moreover, the non-rectangular shape will lead to non-concave value functions with sharp edges at the walls of the corridor. One has to expect that at least the latter will put a strain on the value approximation quality.

Reviewing the results of section 5.2.3, the diversification of the filters in room dependent trigonometric basis functions appear in a new light. Since the covered areas are convex, abrupt changes in the value function appear only \textit{at the contact point} between rooms and therefore filters.

However, since we do not know the optimal SFA responses of the two room environment, we decided to stick to the known artificial responses as described in section 5.3.2. The convergence quality with respect to the number of optimal responses is shown in figure 5.20. Compared to the original task depicted in figure 5.17 one needs much more responses (at least 100) to reach the working regime. Also the convergence quality is much lower, translating in the best cases to ca. 4 unnecessary steps.

To sum it up, the task has proven to be \textit{much} more complicated. Besides, the SFA task is probably harder too, leading to a more distorted state representation. However, we performed a series of tests with preprocessed video images from the simulator, using the first 10 to 500 filters. In terms of convergence quality, no learned control differed much from the baseline in figure 5.20.
5.3.5 Discussion

We successfully conducted the main experiment. Assuming optimal responses, as few as 20 filters are sufficient to learn a near optimal control. Using too much filters, however, produces catastrophic overfitting. Switching to SFA preprocessed video images yields, at least in principle, the same result. However, we need much more filters (at least 80) and the resulting control needs considerably more steps to reach the goal area. Albeit not as well validated as the simulator experiment, our method has proven to work on a real robot as well.

However, both successful experiments based on video images exhibited erratic behaviour at some points. The robot first gets caught or is ”undecided” between left and right rotations but then escapes without obvious reason. Close observation reveals the effect to be present only (but not always) when actions change (in opposition to continuous driving or rotation). At these positions two or more actions must have similar Q-values and noise in the representation can induce erratic behaviour. This kind of behaviour has not been observed using artificial state representations, which supports the conclusion.

5.4 Conclusion

We wanted to give a proof of concept that LSPI can learn a efficient control based only on the video images preprocessed by filters learned by SFA. Given the results of the last section, we can say we have. However, we also demonstrated that with the current computational capacity we can only solve simple problems, yet.

From our analysis we can identify the most likely sources of error:

- **Sensor errors**: Real video images are not constant over time, so the SFA output will always be afflicted by noise. While noise afflicted transitions were always part of the policy iteration framework, up to now noise afflicted state representations received little attention. The effects of this noise appear in form of the discussed ”uncertain” behaviour.

- **Preprocessing errors**: SFA output does not resemble trigonometric polynomials perfectly. This can induce local anomalies and therefore local value estimation errors. For example, the simulated experiment requires much more SFA filters even though sensory noise does not play a role.

- **Approximation errors**: Abrupt changes in the value function (e.g. at walls) can lead to local approximation errors, because the function class at hand can not represent the slope. For example, in the artificial two-room experiment one needs much more optimal responses, due to the tight corridor.

However, the most dangerous source of error is over- and underfitting. While underfitting is simply a question of computational power, overfitting could be lessened by regularization and more training samples.
Chapter 6

Conclusion

6.1 Summary

Applying reinforcement learning methods onto real-world scenarios bears one overwhelming obstacle: The state of the world. The most common mathematical formalism of Markov decision processes (MDP) requires at all times the complete state in a suitable representation. Even if one assumes real-world sensor readings to hold the complete state, its complex and noise afflicted structure is hardly suitable for any learning algorithm.

The most common approach to this problem are hand-crafted heuristics to filter state information out of raw sensor data. However, since unforeseen situations and interactions will occur, this approach is bound to fail outside the controlled conditions of a laboratory. Biological systems, on the other hand, demonstrate the ability to learn efficient representations of their environment. These representations do not only represent the environment well, but can also adapt when conditions change. Thus, faced with real-world scenarios, one should rather learn a representation of sensor data than simply define a heuristic one.

In this thesis we have explored the case of robot navigation. As a handicap, the only accessible state information were the images of a head mounted video camera. We chose a well known reinforcement learning algorithm, least squares policy iteration (LSPI), to learn a navigational control. The only reinforcement signal were a reward in the goal area and a punishment near walls.

LSPI is based on the least squares Q-value algorithm (LSQ), which fits a linear function to approximate the Q-value of all state-action pairs. After learning, the control will choose the action with the highest Q-value in the current state. Given the state in form of the current video image, a linear function is not powerful enough to approximate the Q-value function well.

From approximation theory we know of several sets of basis functions, that are particularly suited to approximate continuous functions by linear weighting. To allow LSPI to learn the task, we therefore must aim for a set of filters that extract the state in the form of suitable basis functions. This thesis is focused on
the unsupervised method of slow feature analysis (SFA), which produces filters that are in the limit equivalent to trigonometric polynomials.

Approach

Assume a static environment in which a wheeled robot can navigate by moving forward and rotating. The only non-static variable is the robot's position and orientation. Since all possible images depend exclusively on these variables they form the complete state. In this environment, we record a random walk in which orientation and position change slowly.

The main principle of SFA, temporal coherence, aims to construct filters that minimize the change in the filtered training set. To avoid trivial solutions, the filters output is bound to change by constraining it to unit variance. Another constraint, decorrelation, ensures a set of orthonormal filters.

Since these constraints force the filtered output to change, the slowest change will follow the state of the random walk. The specific optimization problem employed by SFA leads to trigonometric polynomials as optimal solution, i.e. assuming infinite number of training samples and unrestricted model class.

The main experiment in this thesis consists of an initial random walk video on which we learn a set of filters with SFA. After applying the learned filters onto the initial video, the output is used as input of LSPI. We obtain a linear weighting of filter outputs for every action, which approximates the Q-value. Given a current video image, the control will select the action with the highest Q-value, i.e. that promises the most future reward. In our case that means to navigate as fast as possible into the goal area, since it is the only available reward, while avoiding walls.

Results

We examined two environments. The first was a simple rectangular laboratory area, which was evaluated with a real robot and as a simulation. The second consisted of two quadratic rooms connected by a small corridor. Here we performed only simulated experiments.

In the simulation of the rectangular environment, our method produced controls that differed only around 2 to 3 steps per trajectory from the optimal choices. The real robot also succeeded, but reached the goal only in 80% of the test trajectories and took significantly longer than expected.

The more complicated two-room environment did not yield a working control. However, tests under optimal conditions show that the task is significantly more complex than the former one. It is the authors' belief that with more computational resources in both phases, SFA and LSPI, a successful control can be learned.
6.2 Discussion

After presenting the methodology and results in the last section, we want to discuss some problems the author noticed during his work on this thesis. The discussion will first review general flaws, followed by a close look into detailed problems and some suggestions how to overcome them.

We will pick up some of the topics in the next section to make concrete suggestions on possible future advancements.

Slow feature analysis

Despite the extension to kernel SFA, slow feature analysis still suffers performance issues, as the failure of the two-room experiment shows. However, even if all practical problems can be solved, one has to ask if a task independent preprocessing can handle real scenarios at all.

Without any insight in the task at hand, the extracted basis functions have to cover all state space dimensions and all combinations of them. Given a certain approximation quality in every dimension (e.g. polynomials up to some degree), the number of required filters grows exponentially in the dimensionality of the extracted state space. For example, a trigonometric representation of a p dimensional state space with degrees \((d_1, \ldots, d_p)\) and \(\forall i, j : d_i \approx d_j\) grows exponentially in \(p\). Due to mixtures in all but the first few filters, we cannot exclude unwanted dimensions or combinations, even if we would know them.

Even more, we cannot be certain that the world can be modelled by a finite dimensional state space. A complex system, e.g. a laughing human or a broad-leaved tree in the breeze, would require an inconceivable high dimensionality. Even with a model class that can represent the whole space, the number of required training samples would go against infinity.

Thus, extracting the complete state space is only feasible in very controlled, unique cases. In the end, we would like to extract only the subspace that is useful for the general "class" of problems at hand. For example, if every considered task in some room is independent of the horizontal position, a trigonometric representation of vertical position and orientation would be sufficient for any navigational control. In this context the state space must not represent some underlying "real" causes (e.g. muscle movement) but more problem dependent "meta" causes (e.g. smiling). Section 6.3 will present a more concrete proposal how to achieve this.

- With the exception of the simple case of rectangular rooms, there are no theoretical predictions for optimal responses. Given the variability of environmental states, this can be seen as a major disadvantage. For example, imagine a robot arm with 5 joints. Ideally, one would expect a 5-dimensional combination of free- or cyclic-boundary conditions, but as in the two room case, the arm movement will be constrained by the environment. Therefore the optimal responses will be unpredictable in all
but the most simple cases. However, it is not clear if these unexpected responses will facilitate or limit the filters approximation capability.

- This thesis always assumed the current state of the environment to be encoded in the current video image. Of course, this is not always the case. In line with the simultaneous localization and mapping (SLAM) method, one could include short term memory to track the current position in such cases. However, this would require either a complete reformulation of the optimization problem or a sophisticated post-processing of the SFA output. A much simpler heuristic solution is presented in section 6.3.

### Policy iteration

In the tabular representation, i.e. with small set of discrete states, policy iteration is guaranteed to converge monotonically to an optimal policy. This guarantee, however, does not extend to the realistic case of approximated Q-value functions.

The successive application of a policy estimation and greedy policy improvement step reminds of the expectation maximization algorithm (EM, e.g. [9]). In a discrete version (e.g. K-means, e.g. [5]), this popular algorithm is prone to become stuck at local minima. This effect resembles the results of policy iteration in the unstable regime (see sec. 5.3.2). In difference to policy iteration, for EM a number of probabilistic extensions exist (e.g. soft K-means, e.g. [5]), that greatly reduce (albeit not eliminate) this problem.

However, as the modified initial policy in section 5.3.2 demonstrated, it is possible to use probabilistic choices instead of a pure greedy policy. In section 6.3 we will discuss a consideration of error sources (discussed below) into the policy improvement step. When these problems are discussed in literature, the only considered errors are due to a weak model class. In practice, however, two other sources of error have come to light:

- Every real preprocessing will exhibit some anomalies. The resulting local approximation errors can be amplified by the policy iterations and thus ruin an otherwise good policy.

- Since real sensors are afflicted by noise, the control will exhibit erratic behaviour in areas in which Q-values of the best actions are close by. In the worst case, oscillating behaviour can occur, e.g. turning back and forth.

### Application

At last we have to review the general applicability of the presented algorithms:

- Restricting oneself to discrete actions greatly reduces the area of application. The only way to circumvent this, discretizing continuous actions, increases the number of actions immensely. Because the Q-value estimator LSQ scales cubic in the number of actions, this quickly becomes infeasible.
6.3. OUTLOOK

• Constructing a suitable reinforcement learning scenario is not as intuitive as it might look like. In particular the choice of hyper parameters ($\gamma$, number of filters and amount of reward/punishment) influences the resulting policy considerably.

• The presented method looks promising, but sticks out by its high computational demand. Due to its biological motivation, its computational elegance does not transfer to von Neumann architectures of most modern computers. From this background it looks natural to use parallel processing architectures, e.g. graphic cards, programmable logic arrays or vector processors. Indeed, with these one could consider far more complex models in reasonable time.

However, both SFA and LSPI algorithms are in the presented form not parallelizable. Besides many matrix multiplications, which can be parallelized well in a shared memory architecture, the key elements are matrix inversions or eigenvalue decompositions. There exist parallel versions of both problems, but they are not as efficient and may introduce additional side effects.

In the end, however, the human brain performs these tasks in a massive parallel processed fashion. This alone makes it a promising approach.

6.3 Outlook

As discussed above, application of reinforcement learning to real-world scenarios still bears many problems. The author wants to give here only a small selection of potential improvements, that followed directly from his work on this thesis.

Exclude unwanted states from SFA

To apply the proposed method to non-static environments, one has to exclude unnecessary state subspaces from the SFA solution. Due to mixtures of the optimal responses, one can not directly exclude single filters. Instead, the optimization problem has to include a term that penalizes dependence on unwanted dimensions. It is important that the resulting filters do not specialize too much in the task at hand. For example, in a navigation task a set of filters that support only policies that drive to the center of the room would not work with another goal.

In line with canonical correlation analysis and partial least squares, one possible approach would maximize the correlation of the filters to a target value. As a complication, we do not know a target value directly, but only the experienced reward.
SHORT TERM MEMORY IN PREPROCESSING

A thorough consideration of holding a current state would require a complete reformulation of the SFA optimization problem. However, an easy consideration of the predecessor state (e.g., temporal smoothing $x_t = \eta x_{t-1} + (1 - \eta) \phi_t$) could stabilize the current state estimation. Since the state $x_{t-1}$ depends on all previous observations $\phi_0, \ldots, \phi_{t-1}$, the same position can be represented by different states $x_t$, depending on the past. This will induce additional "noise" in the representation, so the parameter $\eta$ should be chosen very small.

CONSIDER LOCAL ERRORS IN POLICY ITERATION

In section 5.3.2, we introduced a simple modification to the initial random policy of LSPI. Instead of sampling the second action randomly, we considered all actions: $\phi'(x) = \frac{1}{|A|} \sum_{a \in A} \phi(x, a)$. In the following iterations, however, we chose this action greedy. If we review the sources of error from the previous section, we see that these errors are not distributed equally over the state space:

- Weak function classes (e.g., not enough filters) have problems to approximate the slope of abrupt changes in the reward. However, most areas of the value function are smooth enough.

- In areas with similar Q-values noise affected controls will show erratic behaviour. Where Q-values differ enough, the control will be stable.

- SFA filters tend to differ from the optimal responses locally, when the considered function class can not map an image properly.

The first step would be to determine these local errors. With errors and Q-values at hand, one can calculate a realistic probability $p(\cdot)$ for an action to be chosen by a greedy policy. Instead of just choosing one action greedy, one could learn all possible actions at once: $\phi'(x) = \sum_{a \in A} p(a) \phi(x, a)$.

After the experience with the new initial policy, one can hope that the resulting policy iteration will be more stable and therefore converge better.

POLICY DEPENDENT NORM

LSPI is based on the squared $L_2$ norm, which means it aims to distribute the approximation error equally on all training samples. However, as we have seen in our previous discussion, areas with nearby Q-values need much better approximation than those far-off. It would improve the reliability of the control if one would use a policy dependent norm, i.e. put more weight on samples with similar Q-values.
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