

Master Thesis

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BPM

Reinforcement Learning Based Optimization in a Discrete Event Simulation Environment for Optimal Job Assignment in Workflow Processes

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Zurich^{UZH}



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Abstract

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Zusammenfassung

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Introduction

1.1 Problem Definition

Workflows are IT solutions that can help increase efficiency and get tasks done better and faster. However a key element of each workflow process still remains the human aspect. This human aspect can take many facets, such as humans analyzing a process, humans designing a process and humans executing the latter. This thesis focuses on the latter *i.e.*, where human agents interact with the workflow process in order to work on tasks. A business process that has been efficiently analyzed and subsequently optimally implemented still cannot ensure optimal execution, or no optimal execution can be achieved while a human intervention for task execution is present. It is here that optimal role resolution comes in play: optimally choosing and assigning a specific task inside the workflow process to the best possible actor is a non trivial task that has to be solved in order to close the “optimization” circle that workflow engines advertise.

This field is relevant since an optimal role resolution can bring optimization from many sides:

1. cost savings, 2. fairness in workload assignment 3. optimal resources usage.

Currently many different workflow engines exist, ranging from complete fully functional suites and down to extensible frameworks that allow the implementer to adapt it to its own needs. However all these solutions lack optimality in the task assignment sector.

1.2 Objectives

The objectives of these thesis build upon the work of Zeng and Zhao [Zeng and Zhao, 2005], in which they depicted preliminary policies for optimal role resolution, and extends these capabilities from a threefold perspective: 1. further develops the mathematical premises and extends the capabilities of the batching policies proposed by Zeng and Zhao 2. explores the capabilities offered by RL as addition and improvement for even preciser, faster and better task assignment 3. deployment of the aforementioned optimization techniques in an operative environment of a real estate company using a workflow engine.

Formally, this thesis tries to answer the following research questions:

- RQ. 1** Can current optimization methods for job assignment in workflow processes be further developed?
- RQ. 2** Are there state of the art approaches that can complement job assignment with mathematical optimization methods?

1.3 Thesis Structure

This thesis is subdivided in five main chapters:

- Chapter 1 gives an overview of why the chosen topic is relevant, what is the current context of the work and how this work fits in. It moreover articulates the central research questions that permeate this thesis and gives an overview of this essay
- Chapter 2 gives an overview of the most important conceptual definitions and the state of the art literature review in the touched thematic topics of this work. Conclusively this chapter critically reflects upon the existing literature and exposes the deficits that this thesis aims filling
- Chapter 3 gives an overview of the approach used for the research *e.g.*, the analysis environment and the used tools, states the hypothesis that wants to be proved and eventually describes statistically and qualitatively the data sets upon which the methodology is applied
- Chapter 4 builds upon Chapter 3 and makes its way into the hypothesis test field and the respective analysis results. Furthermore looks introspectively on the data correlation and gives an interpretation of the latter. Eventually in this section a statement about the contribution that the results bring into this field is given
- Chapter 5 is the culminating chapter in which a summary of the key findings of the thesis are outlined, the research questions posed in Section 1.2 are answered by looking at the actual usability, limitations and to whom the results are most applicable. Finally outlooks about the future trends and how the empirical results of this thesis can be extended by prospective researchers.

Theoretical Foundations

2.1 Literature Overview

This section serves as an overview of the state of the art literature that exists and has been used as a foundation basis for this work and is divided in different thematic subsections. For a graphical representation of the literature overview mindmap refer to Figure A.1.

2.1.1 Queueing

Queueing is a topic that talks about how people or more general agents are to be served while waiting (*i.e.*, queueing) inside a system.

Starting with one of the most notable contributions to this field done by Kendall and his work on the Markov chains in queueing theory, where he formally defines different types of queues [Kendall, 1953].

Pinedo outlines in his work the most prominent key metrics that can be used in order to assert and measure queues performance [Pinedo, 2008].

Adan and Reising describe the necessary basic concepts for queueing theory: statistical foundations outlined in their work about different modeling techniques for randomized generation rates, such as the Erlang's distributions which serves as backbone for this thesis [Adan and Resing, 2016].

2.1.2 Workflow

Baker formally defines the KPI used by Zeng and Zhao in their work for evaluating their policy efficacy, called task flowtime [Baker, 1974].

Another good starting point in the workflow thematic is Macintosh's work in which he gives an overview of the five levels of process maturity [Macintosh, 1993]: 1. Initial, the process has to be set up 2. Repeatable, the process has to be repeatable 3. Defined, documentation standardization of processes 4. Managed, measurement and control of processes 5. Optimizing, continuous process improvement

Georgakopoulos *et al.* give a comprehensive business oriented overview of the different workflow technologies present on the market used as a sound foundation for analyzing the present technologies [Georgakopoulos et al., 1995].

On this note, Giaglis lays out four different process perspectives: 1. Functional 2. Behavioral 3. Organizational 4. Informational.

His framework focuses on three dimensions: 1. Breadth, where modeling goals are typically addressed by technique 2. Depth, where modeling perspectives are covered 3. Fit, where typical project to which techniques can be fit.

The presented framework is used to combine the three different dimensions in order to assert a possible best fit of a specific modeling technique based on which approach to be used under the constraints of a modeling perspective to cover [Giaglis, 2001].

Mentzas *et al.* focus on a qualitative level on how workflow technologies can facilitate implementation of business processes by focusing on the pros and cons of adopting alternative workflow modeling techniques [Mentzas et al., 2001]. Moreover they formally define what a workflow management system is and subdivide it in three main categories: 1. Process modeling 2. Process re-engineering 3. Workflow implementation and automation.

Each level of maturity as defined by Macintosh requires a different model, such as the first three levels might require more descriptive models whereas levels four and five require decision support keen models in order to monitor and control processes [Mentzas et al., 2001].

Aguilar-Savén describes the main modeling techniques existing with workflow being one of them [Aguilar-Savén, 2004].

Interestingly enough, workflow implementation in real world cases is not always only coupled with directly measurable effects, sometimes even unexpected results happen. What is called the “workflow paradox” according to Reijers and van der Aalst is the fact that the very fact of companies accepting requests for workflow introduction might actually be the most promising way that leads to potentially better and more suitable alternatives [Reijers and van der Aalst, 2005].

The key core topics on which this thesis lays its foundations upon is the work done by Zeng and Zhao: effective role resolution *i.e.*, the mechanism of assigning tasks to individual workers at runtime according to the role qualification defined in the workflow model [Zeng and Zhao, 2005], is the core aspect that is being extended during this thesis work.

Zeng and Zhao differentiate between staffing decisions and role resolution, with the former being the assignment one or more role to each user and the latter being the assignment of a specific task to an appropriate worker at runtime [Zeng and Zhao, 2005]. Staffing decisions are usually made off-line and periodically, thus being more of a strategic nature [Zeng and Zhao, 2005]. If role resolution were to be made on-line it could translate to a major operational level decision *i.e.*, the differentiation between strategic vs. operational playing role [Zeng and Zhao, 2005].

They moreover define three roles a workflow can fulfill [Zeng and Zhao, 2005]: 1. System built-in policies 2. User customizable policies 3. Rule based policies.

Considering capacities of resources restrictions under the assignment problem is an NP-hard computational problem and Zeng and Zhao focus on how to solve the assignment problem and scheduling decisions with consideration of worker’s preferences [Zeng and Zhao, 2005]. For this purpose they define five workflow resolution policies: 1. LLQP 2. SQ 3. K-Batch 4. K-Batch-1 5. 1-Batch-1

For all batch policies a simplified version of DMF has to be solved [Zeng and Zhao, 2005].

Zeng and Zhao’s key findings are outlined as follows [Zeng and Zhao, 2005]: 1. Batch policies are to be used when system load is medium to high 2. Processing time variation has major impact on system performance *i.e.*, higher variation favors optimization based policies 3. Average workload and workload variation can be significantly reduced by online optimization 4. 1-Batch-1 online optimization policy yields best results in operational conditions.

On a detailed note, data flow inside workflow processes has to consider possible anomalies that might happens and this aspect has been extensively studies by Sun *et al.* where they formally define data flow methodologies for detecting such anomalies [Sun et al., 2006]. Their framework is divided in two components: 1. Data flow specification 2. Data flow analysis.

Mentions that simulations for workflow management systems is usually inefficient and inac-

curate arises yet again [Sun et al., 2006]. They moreover discuss aspects that data requirements have been analyzed but the required methodologies on discovering data flow errors have not been extensively researched [Sun et al., 2006].

A more recent taxonomy of different Business Process Management (BPM) application is given by a collaboration between SAP and accenture [Evolved Technologist, 2009].

An analysis of the Critical Success Factors (CSFs) for BPM is required in order to assert a product validity and this has been done by Trkman where he defines CSFs from three perspectives [Trkman, 2010]: 1. Contingency theory 2. Dynamic capabilities 3. Task-technology fit theory.

The domain of workflow processes and engines is permeated by Business Process Model and Notation (BPMN) and Silver's guidelines are excellent formal foundations [Silver, 2011].

Change management in workflow is yet another interesting aspect that should be considered and this has been broadly studied by Wang and Zhao where they developed an analytical framework for workflow change management through formal modeling of workflow constraints [Wang and Zhao, 2011].

In companies different types of workflow models can exist and Fan *et al.* focus on two of these [Fan et al., 2012], namely: 1. Conceptual 2. Logical.

Conceptual models serve as documentation for generic process requirements whereas logical models are used as definitions for technology oriented requirements [Fan et al., 2012]. One difficult aspect is the transition from the former to the latter and Fan *et al.* propose a formal approach to efficiently support such transitions [Fan et al., 2012].

Sun and Zhao cover the aspect of formal analysis for workflow models and they claim that it should help "alleviating the intellectual challenge faced by business analysts when creating workflow models" [Sun and Zhao, 2013].

2.1.3 Reinforcement Learning

RL is a branch of machine learning that promises to overcome the drawbacks posed by the latter by not requiring a training set for efficient machine decisions [Sutton and Barto, 2017].

One of the first MC based Policy Gradient (PG) methods is the algorithm proposed by Williams called REINFORCE [Williams, 1992].

Vanishing Gradient Problem (VGP) states that even very large change in partial derivatives on initial layers have imperceptible effects on subsequent layers, as outlined by Bengio *et al.*, which is a problem that affects deep ANNs [Bengio et al., 1994].

Haykin's comprehensive work on ANNs is an excellent theoretical foundation which serves as basis for critical concepts regarding the matter [Haykin, 1998].

Theoretical definition on deep ANNs is also given by Lecun *et al.* which was used to better understand more recent developments in this domain [Lecun et al., 1998].

PG methods with VFA and their convergence is of vital importance and according to Sutton *et al.* this can be achieved by representing the policy by an own function approximation which is independent of the value function and it is updated according to gradient of the expected rewards with respect to the afore mentioned policy [Sutton et al., 1999].

Another branch originated from RL is Inverse RL (IRL): Ng and Russell outline the required algorithms for this domain [Ng and Russell, 2000].

Discretization of the state action space is not always feasible and different techniques have to be used for tractability [Smith, 2002]. Smith proposes such an approach which he calls "self-organizing map" [Smith, 2002].

Abbeel and Ng collaboration lays the basis from a bleeding edge branch of IRL called Apprenticeship Learning (AL), which trains policies without rewards function by merely observing "expert" agents performing a task in a specific domain [Abbeel and Ng, 2004].

Bengio further develops the foundations laid by Lecun and expands the theoretical basis of deep ANNs [Bengio, 2009].

Statistical identifiability in RL is a crucial aspect that has to be ensured for effective learning, as were it not the case RL update methods might remain stuck in suboptimal solutions and never converge, as explained by [Zhang and Hyvärinen, 2011].

Yet another problem in which deep ANNs might incur in addition to VGP is the so called Exploding Gradient Problem (EGP) as defined by Pascanu *et al.* [Pascanu et al., 2012].

This huge state space requirement is a clear limitation to lookup tables [Sutton and Barto, 2017]. Even if memory would not be a constraint, the actual learning from such tables would be infeasible [Sutton and Barto, 2017]. In order to pragmatically learn by reinforcement on such huge problems, VFA in the domain of RL proves to be a viable solution [Sutton and Barto, 2017]. For different types of RL approaches *i.e.*, MC or TD methods exist different types of VFA, ranging from simple linear combinations of features for MC to ANNs for TD learning [Sutton and Barto, 2017]. All these different methodologies are outlined in the tutorial by Geramifard *et al.* [Geramifard et al., 2013] and complement the theoretical foundations laid by Sutton and Barto.

Overfitting for deep ANNs is a common problem [Sutton and Barto, 2017, p. 218]. Srivastava *et al.* propose the dropout method which proves to be a domain standard in regards to this problem [Srivastava et al., 2014].

As Markov Decision Processes (MDPs) grow in size, so does the required computational memory to solve possible discrete lookup tables modeling the state-actions spaces that characterizes them [Sutton and Barto, 2017]. Notable examples that show how large some of the most common problems can be [Sutton and Barto, 2017]: 1. the game of backgammon has a total of 10^{20} states 2. the traditional Chinese abstract board game Go has an estimated total of 10^{170} states 3. flying a helicopter or having a robot move in space all require a continuous state space.

When working with on-line algorithms such as TD it is important to choose correct parameters for an effective learning process, otherwise the learning algorithm put in place might never converge towards an optimal solution [Sutton and Barto, 2017]. This aspect is being discussed by Korda and Prashanth in which they depict different non-asymptotic bounds for the TD learning algorithms [Korda and Prashanth, 2014].

There are two main fields in RL, one is using VFA for either the state value function or for using control mechanisms with the state Action Value (AV) function, while the other one is using PG methods for policy optimization [Sutton and Barto, 2017]. The latter offers different methods such as the naive finite difference methods, MC based PG methods and finally Actor Critic (AC) PG methods as defined by Silver *et al.* [Silver et al., 2014].

Clevert *et al.* discuss a special class of activation functions for ANNs called Exponential Linear Units (ELUs) which are improvements over classical Rectified Linear Units (ReLUs) [Clevert et al., 2015]. ELUs activation functions are used for the modeling of the ANNs layers in this thesis.

Gershman proposes further advancements to Zhang's work on statistical identifiability [Zhang and Hyvärinen, 2011] by analyzing prior distributions of the parameters [Gershman, 2016]. He argues that his approach helps to some extent to overcome the identifiability problem [Gershman, 2016].

Notable works in the field of RL and its application include Google DeepMind work on novel algorithms for tackling fields previously barely scratched, as mentioned by Mnih *et al.* and Silver *et al.* [Mnih et al., 2015, Silver et al., 2016].

Sutton and Barto started working on the RL topic in the early nineties and are now planning their third edition of the famous book on machine learning, which is due in 2017 [Sutton and Barto, 2017]. In our case RL is used in order for the policies to be able to improve themselves by continuously analyzing their own decision models and optimize upon them. Their work is the backbone used for this thesis for the RL domain.

2.1.4 Optimization

Dynamic allocation of jobs to users, or how Zeng and Zhao define it *i.e.*, DMF [Zeng and Zhao, 2005], is a problem that is NP-Hard, as demonstrated by Garey and Johnson [Garey and Johnson, 1990].

Under mathematical optimization or specifically to the domain of the thesis, a mixed integer optimization problem must be solved in order to optimally assign jobs to users in the workflow processes. The generalized assignment problem is a very well known problem in combinatorial mathematics and Cattrysse and Wassenhove give an overview of different algorithms for solving the generalized assignment problem [Cattrysse and Wassenhove, 1992]. Heuristics are also a viable solution for solving such adaptation of the generalized assignment problem, as Racer and Amini state [Racer and Amini, 1994]. Moreover a global perspective of optimization from a mathematical perspective is given in Boyd and Vandenberghe's work on convex optimization [Boyd and Vandenberghe, 2004].

Last but not least, according to the AIMMS guidelines, there are different linear programming tricks that can be used to shape such problems in solvable outlines [Bisschop, 2016]. In this thesis, a specific linear programming trick, called either-or constraints, was used by adding so called auxiliary variables to the evaluation method presented in order to efficiently solve an otherwise non solvable equation [Bisschop, 2016, p. 77].

2.1.5 Simulation

Bahouth *et al.* focus on algorithmic analysis of discrete event simulation supplemented with focus on factors such as compiler efficiency, code interpretation and caching memory issues [Bahouth et al., 2007]. According to their findings, a significant speedup can be achieved if one addresses the afore mentioned facets [Bahouth et al., 2007].

Simulating queues can prove to be arduous [Matloff, 2008]. The main differentiation needed here is that between continuous and step functions: the former is the result when the events being simulated yield values that if plotted against the simulation time give a continuous function [Matloff, 2008]. On the other hand, if we simulate events that yield discrete values, such as inventory changes in a storage facility and plot the results against the simulation time we would get so called step functions [Matloff, 2008].

According to Matloff, different world views for discrete event programming [Matloff, 2008], as he calls them paradigms [Matloff, 2008]: 1. Activity oriented 2. Event oriented 3. Process oriented.

Activity oriented can be summarized as simulation events where time is being subdivided in tiny intervals at which the program checks the status for all simulated entities [Matloff, 2008]. Since petite subdivisions of time are possible in such types of simulations, it is clear that the program might prove tedious, since most of the time there won't be any change in state for the simulated entities [Matloff, 2008]. Event oriented circumnavigate this issue by advancing the simulation time directly to the next event to be simulated [Matloff, 2008]. By filling these gaps, a dramatical increase in computation can be observed [Matloff, 2008]. Last but not least, the process oriented simulation models each simulation activity as a process or thread [Matloff, 2008]. Management of threads has steadily decreased in today's computation since many different packages for governing such tasks exist [Matloff, 2008].

Methodology

3.1 Analysis Structure

3.1.1 Tools

Different tools were used in the analysis environment in order to efficiently simulate and analyze the work of this thesis.

The whole architecture is subdivided as follows: 1. The simulation environment is based on Python 3.5.2¹ using the Anaconda² platform and as a discrete event simulation the SimPy 3.0.10³ package is used. 2. The resulting data are interpreted and analyzed using Python and its plotting library: Matplotlib 2.0.0⁴. 3. Tensorflow 1.0⁵ is the library used for the neural networks modeling. 4. Coding was done using PyCharm 2017.1⁶ as IDE for Python. 5. For solving the mixed integer problems for batching policies Gurobi 7.0.1⁷ was used.

3.1.2 Discrete event simulation using SimPy

SimPy is a Python process-based discrete-event simulation framework. It exploits Python generators according to which it models its processes.

Active components such as agents in a workflow are modeled as processes which live inside an environment and the interaction between them happens via events.

As previously mentioned, processes in SimPy are described by Python generators. During their lifetime they create events `yield` (Note that with the term `yield` here it is to be understood as Python's `yield` statements)⁸ them to the environment, which then wait until they are triggered. The important logic to understand here is how SimPy treats yielded events: when a process yields an event it gets suspended. From the suspended state a process gets resumed when the event actually occurs (or in SimPy's notation when it gets triggered).

SimPy offers a built-in event type called `Timeout`: events of this type are automatically triggered after a determined simulation time step. Consistency is asserted since a timeout event are created and called by called the appropriate method of the passed `Environment`.

¹<https://www.python.org> (accessed: 06.01.2017)

²<https://www.continuum.io/anaconda-overview> (accessed: 03.04.2017)

³<https://simpy.readthedocs.io/en/latest/> (accessed: 06.01.2017)

⁴<http://matplotlib.org/> (accessed: 03.04.2017)

⁵<https://www.tensorflow.org/> (accessed: 03.04.2017)

⁶<https://www.jetbrains.com/pycharm/> (accessed: 03.04.2017)

⁷<http://www.gurobi.com> (accessed: 06.01.2017)

⁸https://docs.python.org/3.5/reference/simple_stmts.html#the-yield-statement (accessed: 06.01.2017)

3.1.3 Analysis Environment

The analysis environment consists in an object-oriented implementations of workflow process elements such as user task, starting, decision and end nodes which have been developed to allow the simulation framework to effectively run. This object-oriented exoskeleton implementation of the workflow elements can be seen depicted in Figure 3.1.

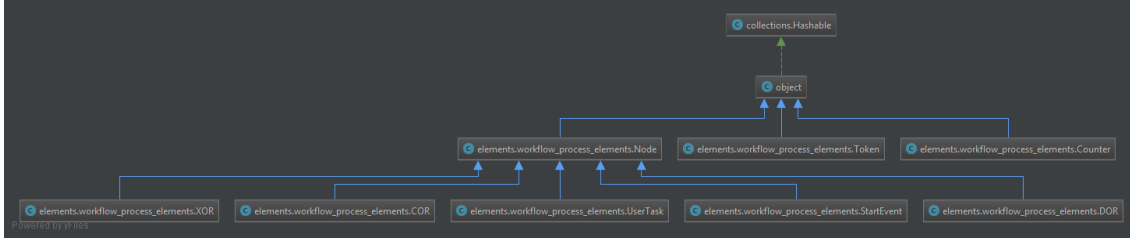


Figure 3.1: Workflow elements

The core elements of a workflow process (relevant for the simulation environment) are start nodes, user tasks, decision nodes and end nodes. Start events are used to indicate where and how a process starts and usually each process has only one such event [Silver, 2011, p. 42]. No distinction between trigger types is being made.

Start event

Start event objects require a simulation environment, a generation interval, an actions to follow array and its corresponding weights. The generation interval is generated in a three step process: 1. before the simulation starts, a fixed service interval time unit s , number of users n and an average system load l are set. In contrast to Zeng and Zhao’s work, where the generation λ interval follows a Poisson distribution [Zeng and Zhao, 2005] and is defined as shown in Equation 3.1, here the generation interval is a plain scalar value. 2. for a Poisson random exponential sampling of the generation rate, NumPy’s implementation of its exponential distribution is used⁹.

$$\lambda = \frac{ln}{s} \quad (3.1)$$

The actions to be followed are also defined in a two step process: 1. a per workflow process action pool is defined a priori in order to assert that tokens navigate the process in a “semantically correct” fashion 2. then a weights vector is defined which assigns a weight to each possible action path to the actions pool.

Such an approach allows to fine tune how often tokens will follow a predefined path along the process in order to efficiently simulate and put under stress specific paths of the process.

In order to assert fairness among all simulation runs a master random state is assigned to the start event. This master random state is generated from the PCG family of random generators which exhibit peculiar characteristics, one amongst all is the possibility of “jumping ahead” in the state. By such means of ahead jumps it is possible to assign a fixed number of random yet consistent choices among all runs, since each generated token receives from the start event a

⁹<https://docs.scipy.org/doc/numpy/reference/generated/numpy.random.exponential.html> (accessed: 06.01.2017)

“jumped” copy from the master state. For a better overview of the characteristics of the PCG random generators family consult its official outline ¹⁰.

Even though tokens are generated infinitely, this process is controlled from the simulation environment where a discrete simulation time steps have to be set, as it can be seen from Listing 3.1.

This can be interpreted as that the whole simulation will persist for 100 time steps and it will then stop when the internal clock reaches 100. Please note that events that have been scheduled for time step 100 will not be processed. The logic is similar to a new environment where the clock is zero and no event have been processed yet.

```
# "global" variables
SIM_TIME = 100
# runs simulation
env.run(until=SIM_TIME)
```

Listing 3.1: Starting the simulation with discrete time steps

User task

User task objects also require a simulation environment, a policy, a descriptive name, a service interval and task variability. Each user task has a unique `child` field which is being set prior to starting the simulation.

In regards to parameters service interval and task variability a detailed explanation is required. Both are used to randomly sample service rate intervals for each user active during the simulation. Zeng and Zhao in their work follow a two way process to generate such intervals [Zeng and Zhao, 2005, p. 8]. However in this thesis’ implementation a refined version of this process is used: 1. at initialization time, each user task receives a service rate s and a task variability t value 2. inside the policy request method, for each user task a sample of an average processing time following an Erlang distribution (a special case of the gamma distribution) which takes as input parameters a shape k and a scale θ is made. The shape value k , as the name suggests, defines the curve shape that the Erlang distribution will follow. In this case both values k and θ are dynamically evaluated at runtime as $k = s/t$ and $\theta = t$. This concept is depicted in Listing 3.3 3. the average processing time becomes a unique value of each user task object and is used by each policy to sample each user’s service time, again from an Erlang sampled pool as depicted in Listing 3.2 and we shall call this value p_j

Listing 3.2 gives a glimpse of the inner logic of how policies work. It is however out of scope for this section to cover this aspect and it is provided “as is”. For each user eligible to work the assigned token, its service rate is sampled following the Erlang distribution. This time, the Erlang distribution takes as parameters the unique average processing time p_j of user task j and a value worker variability, which is a unique property of each policy, which we shall call w .

In order to sample a service rate p_{ij} following the Erlang distribution for each user i , shape k is evaluated as $k = p_j/w$ and scale as $\theta = w$ as it can be seen in Listing 3.2

```
def request(self, user_task, token):
    average_processing_time = token.random_state.gamma(
        user_task.service_interval ** 2 / user_task.task_variability,
        user_task.task_variability / user_task.service_interval)

    policy_job.service_rate = [token.random_state.gamma(
        average_processing_time ** 2 / self.worker_variability,
```

¹⁰<http://www.pcg-random.org/> (accessed: 03.04.2017)

```

        self.worker_variability /
        average_processing_time) for
    _ in range(self.number_of_users)]

```

Listing 3.2: User service rate sampling following an Erlang distribution

As previously mentioned, the Erlang distribution is a special case of the Gamma distribution where k defines the shape of the curve. This distribution is better suited to model service rates since with an appropriate k one can approximate a normal distribution without incurring in the aspect of having to manually reset negative values to one (thus loosing statistical generality). This is asserted by the formal definition of Erlang's support with $x \in [0, \infty)$.

NumPy's implementation of its Erlang distribution is used¹¹. Equation 3.2 defines the probability density function of the Erlang's distribution with the alternative parametrization that uses μ instead of λ as scale parameter, which is its reciprocal. This corresponds to the NumPy's implementation.

$$f(x; k, \mu) = \frac{x^{k-1} e^{-\frac{x}{\mu}}}{\mu^k (k-1)!} \text{ for } x, \mu \geq 0 \quad (3.2)$$

Each user task object has a claim token method, which takes tokens as input parameters and finally makes a call to its designed policy, passing the token. On this top level, without stepping into the single policies implementations, the logic is straightforward: start events generate tokens, user tasks that are direct children of start events claim the newly generated tokens, ask the designated policies to work the token assigned to them and finally, after a service interval timeout which corresponds to the user's specific service interval, they release the token. The logic can be seen in Listing 3.3.

```

def claim_token(self, token):
    token.worked_by(self)
    policy_job = self.policy.request(self, token)
    service_time = yield policy_job.request_event
    yield self.env.timeout(service_time)
    self.policy.release(policy_job)

```

Listing 3.3: User task claim method

Policy

Policies are a particular object that does not directly participate in the workflow processes, it merely serves a role as a general supervisor that has the whole overview of the process allowing it to operate on a more abstract level.

The implementation of the policy objects can be seen in Figure 3.2.

Each policy is a blueprint for the actual implementation of the policy itself. It holds minimal information such as a simulation environment, number of users and worker variability. The worker variability is a global parameter that is used for the service time generation as already explained in Subsection 3.1.3.

As a blueprint, each policy object defines two abstract method for requesting an optimal assignment for a specific token and for later releasing that token and effectively freeing the user that was busy working on it. Refer to Figure 3.3 for its implementation overview.

¹¹<https://docs.scipy.org/doc/numpy/reference/generated/numpy.random.gamma.html> (accessed: 06.01.2017)

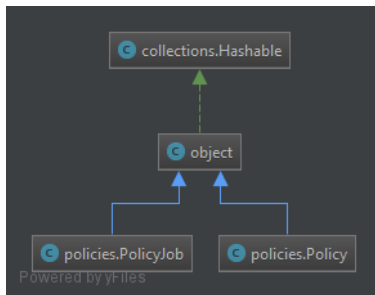


Figure 3.2: Policies abstract implementation

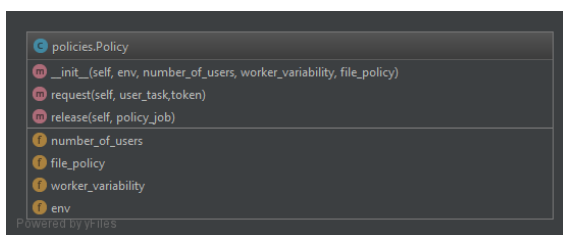


Figure 3.3: Policy methods and attributes

In its request method, each policy generates a policy job object, which is again an abstract implementation of a job that the policy will work in order to return an optimizes assignment to a user task. Each policy job requires a user task and a token object as initialization parameters in order to be uniquely identifiable inside the whole process. Moreover, each policy job object serves as a bookkeeping agent by storing and dumping useful information every time it status changes, such as arrival, assigned, started and finished times, assigned user and a list of service times for all available users. Refer to Figure 3.4 for its implementation overview.

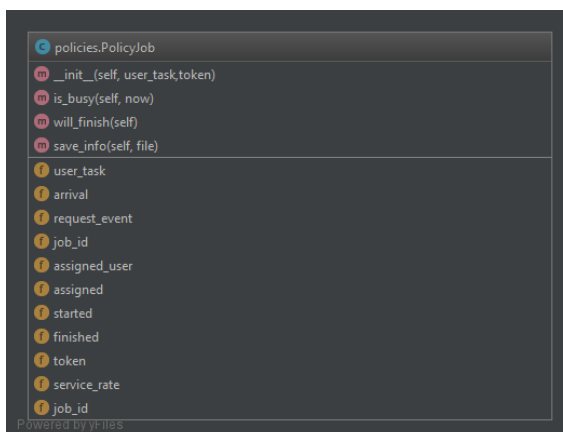


Figure 3.4: Policy job methods and attributes

3.2 Optimization Policies

Different types of policies have been implemented following the foundations laid by Zeng and Zhao as outlined in Subsection 2.1.2. In their work the authors investigate five “role-resolution” policies used for optimal task to user assignment [Zeng and Zhao, 2005, p. 7]. Following a brief description of the five aforementioned policies: 1. A load balancing policy consists in assigning a task as soon as it arrives to a qualified worker with the shortest task queue at that moment. In this policy workers execute tasks assigned to them on a FIFO fashion. The authors call this policy the “LLQP”. 2. A policy that maintains a single queue being shared among all users is referred to the authors as “SQ”. 3. Another policy that maintains both a SQ among all users and each user having an own queue and transfers tasks from the former to the latter is called “K-Batch” policy. Transfer of tasks from the SQ to users is done using an optimal task assignment procedure as soon as the SQ reaches a critical batch size K . 4. The following policies takes the “K-Batch” policy but reduces the individual queue size of each user to one. This means that the optimization problem is still being solved as soon as the SQ reaches the critical size K , however actual movement of tasks from the SQ to the individual user queue happens only when user i is not busy *i.e.*, his individual queue is empty at simulation time t . This policy is called according to the authors as “K-Batch-1”. 5. The last policy further simplifies the fourth by weakening the batch size constraint and reduces it to one. This means that the optimal task assignment procedure is executed immediately. This policy is referred by the authors as “1-Batch-1”.

All batching policies require the solution of an optimization problem. The authors define this problem as “minimizing the maximum flowtime given the dynamic availability of the workers” and call it “MSA” [Zeng and Zhao, 2005, p. 7]. The authors define the task flowtime as the elapsed simulation time between task generation and its completion [Zeng and Zhao, 2005, Baker, 1974]. Formally MSA is formulated as follows:

$$\min_z \quad z \quad (3.3)$$

subject to:

$$\sum_{i \in W} x_{ij} = 1 \quad \forall j \in T \quad (3.4)$$

$$a_i + \sum_{j \in T} x_{ij} p_{ij} \leq z \quad \forall i \in W \quad (3.5)$$

$$x_{ij} \quad \text{or} \quad x_{ij} = 1 \quad \forall i \in W, \forall j \in T \quad (3.6)$$

All variables definition still hold without loss of generality as defined by the authors [Zeng and Zhao, 2005, pp. 5-7].

The class inheritance structure of the policies implementation can be seen in Figure 3.5.

The authors definition of the MSA problem is however a simplified version of the actual problem of “minimizing the maximum task flowtime” (MF) as defined by Baker [Baker, 1974] with consideration of the dynamic arrival of tasks problem, defined by the authors as the DMF problem [Zeng and Zhao, 2005]. The DMF problem is formally defined by Zeng and Zhao as follows:

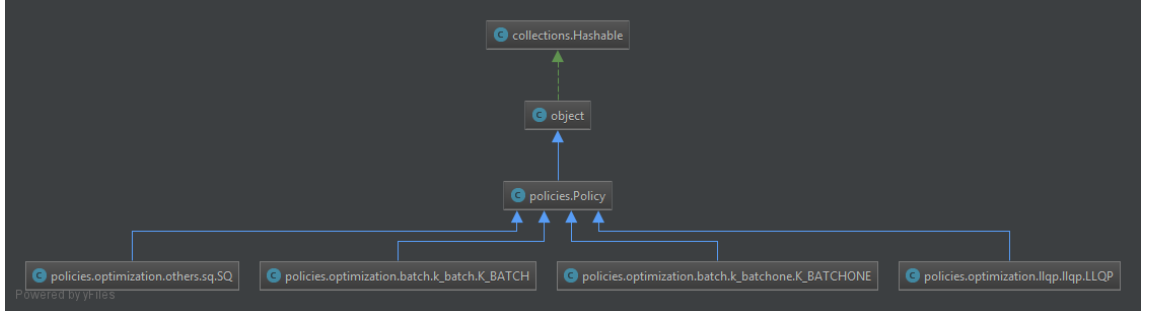


Figure 3.5: Policies class structure

$$\min_z z \quad (3.7)$$

subject to:

$$\sum_{i \in W} \sum_{k \in T} x_{ijk} = 1 \quad \forall j \in T \quad (3.8)$$

$$s_j \geq r_j \quad \forall j \in T \quad (3.9)$$

$$(x_{ijk} + x_{ij'(k+1)} - 1)(s_j + p_{ij}) \leq s_{j'} \quad \forall i \in W, \forall k \in T, \forall j \in T, \forall j' \in T \quad (3.10)$$

$$s_j + \sum_{i \in W} \sum_{k \in T} p_{ij} x_{ijk} - r_j \leq z \quad \forall j \in T \quad (3.11)$$

$$x_{ijk} = 0 \quad \text{or} \quad x_{ijk} = 1 \quad \forall i \in W, \forall j \in T, \forall k \in T \quad (3.12)$$

$$s_j \geq 0 \quad (3.13)$$

Again, all variables definition still hold without loss of generality as described by the authors [Zeng and Zhao, 2005, p. 6]. As Zeng and Zhao note in their work, Equation 3.10 contains nonlinear constraints but mention that by adding auxiliary variables the aforementioned DMF formulation can be effectively converted into a mixed integer program and thus solve it [Zeng and Zhao, 2005, p. 6]. On this note they argue that the application of the DMF problem in practice poses some problems [Zeng and Zhao, 2005]. In this thesis however a conversion of the DMF formulation proposed by Zeng and Zhao is formulated in order to adequately solve the optimization problem. The formal definition of such optimization problem is called EDMF and is devised as follows:

$$\min_{z_{\max}} z_{\max} \quad (3.14)$$

subject to:

$$\sum_{i \in W} \sum_{k \in T} x_{ijk} = 1 \quad \forall j \in T \quad (3.15)$$

$$a_i + \sum_{j \in T} p_{ij} x_{ijk} \leq z_{i*k} \quad \forall i \in W, \forall k \in T \quad \text{for } k = 0 \quad (3.16)$$

$$z_{i*k-1} + \sum_{j \in T} p_{ij} x_{ijk} \leq z_{i*k} \quad \forall i \in W, \forall k \in T \quad \text{for } k > 0 \quad (3.17)$$

$$z_{i*k} + \sum_{j \in T} w_j x_{ijk} \leq z_{\max} \quad \forall i \in W, \forall k \in T \quad (3.18)$$

$$\sum_{j \in T} x_{ijk} \leq 1 \quad \forall i \in W, \forall k \in T \quad \text{for } k = 0 \quad (3.19)$$

$$\sum_{j \in T} x_{ijk} \leq \sum_{j \in T} x_{ijk-1} \quad \forall i \in W, \forall k \in T \quad \text{for } k > 0 \quad (3.20)$$

$$z_{i*k} \geq 0 \quad \forall i \in W, \forall k \in T \quad (3.21)$$

This formulation clearly gets rid of the nonlinear constraints while still accounting for dynamical arrival of tasks, making thus the DMF problem as defined by Zeng and Zhao effectively solvable.

When considering the minimization of the maximum flowtime of a task inside a process, the EDMF formulation can be further simplified by adopting some assumptions about the order and sequence of tasks. Based on how the batching policies are implemented, the policy job objects to be worked by users are implicitly stored in a sorted fashion. This means that the z helper variables defined for EDMF are not strictly necessary and thus can be compressed by Equation 3.22:

$$a_i + \sum_{t=1}^k \sum_j (p_{ij} + w_j I(t=k)) x_{ijt} \quad (3.22)$$

The whole concept consists in the introduction of an identity variable I which is true only if task j is currently being assigned as the k th task to user i , meaning that for this specific case also the waiting time for task j has to be accounted for. For all other cases *i.e.*, $j < k$ the identity variable I will not hold thus effectively zeroing the w_j variable.

Figure 3.6 depicts the potential scenario where three tasks are assigned to a specific user i following a sequence where task 2, 3 and j are assigned respectively as first, second and third tasks (thus respecting the k notation outlined above them).

In order to calculate z_{ijk} , one has to consider also when user i will actually be available to process his first task. This is depicted by the variable a_i , which summed together with the respective service times of user i for task j gives the complete work time user i will require to process all tasks assigned to him.

Without further ado, the simplified formulation of EDMF (called SDMF) is the following:

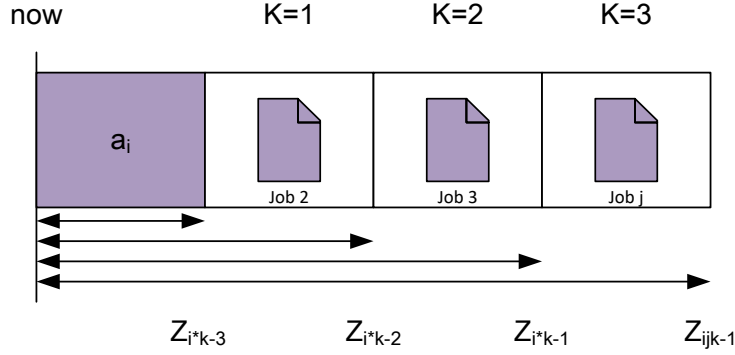


Figure 3.6: EDMF Task Assignment

$$\min_{z_{\max}} z_{\max} \quad (3.23)$$

subject to:

$$\sum_{i \in W} \sum_{k \in T} x_{ijk} = 1 \quad \forall j \in T \quad (3.24)$$

$$a_i + \sum_{t=1}^k \sum_j (p_{ij} + w_j I(t=k)) x_{ijt} \leq z_{\max} \quad (3.25)$$

$$\sum_{j \in T} x_{ijk} \leq 1 \quad \forall i \in W, \forall k \in T \quad \text{for } k = 0 \quad (3.26)$$

$$\sum_{j \in T} x_{ijk} \leq \sum_{j \in T} x_{ijk-1} \quad \forall i \in W, \forall k \in T \quad \text{for } k > 0 \quad (3.27)$$

By comparing both formulation it is clear that SDMF manages to simplify the mathematical formulation and relaxing the required amount of constraints while still attaining the same level of effectiveness. Please note, however, that this simplification is only possible because of the nature of the implementation.

Based on this approach and by further exploiting the implicit order implementation of task arrival in the global queues for both batching policies, it is possible to argue that the k sequence indexing can be relaxed as well, thus even further simplifying the mathematical formulation and respectively the optimization problem size and computation costs.

The formulation of the DMF problem by relaxing both the z variables and k indexes, it is possible to formulate the same DMF problem as follows:

$$\min_{z_{\max}} z_{\max} \quad (3.28)$$

subject to:

$$\sum_{i \in W} x_{ij} = 1 \quad \forall j \in T \quad (3.29)$$

$$a_i + \sum_{k=1}^j (p_{ik} + w_k I(k=j)) x_{ik} \leq z_{\max} \quad (3.30)$$

This formulation is colloquially called ESDMF.

This version is however only possible by the nature of its implementation. Since the both the global as well as the local queues are implemented as FIFO queues, it is possible to relax the ordering constraint from the mathematical formulation since it is already implicitly defined by the implementation.

Yet one last optimization of the method proposed by Zeng and Zhao done in this thesis is a method that aims to optimally solve the assignment problem by changing its goal: minimize the service times by setting an upper bound on the maximum flowtime and is called ST. This method uses a two step process in order to optimally solve the assignment problem: 1. optimally solve by means of using on of the DMF optimization methods previously outlined. This yields an upper bound for the maximum flowtime. 2. use this upper bound as a constraint for the actual optimization in order to effectively optimize the problem for the minimal service time amongst users, jobs and their corresponding service time.

$$\min_z \sum_{i \in W} \sum_{k \in T} z_{ik} \quad (3.31)$$

subject to:

$$\sum_{i \in W} \sum_{k \in T} x_{ijk} = 1 \quad \forall j \in T \quad (3.32)$$

$$a_i + \sum_{j \in T} p_{ij} x_{ijk} - M(1 - \sum_{j \in T} x_{ijk}) \leq z_{i*k} \quad \forall i \in W, \forall k \in T \quad \text{for } k = 0 \quad (3.33)$$

$$z_{i*k-1} + \sum_{j \in T} p_{ij} x_{ijk} - M(1 - \sum_{j \in T} x_{ijk}) \leq z_{i*k} \quad \forall i \in W, \forall k \in T \quad \text{for } k > 0 \quad (3.34)$$

$$z_{i*k} + \sum_{j \in T} w_j x_{ijk} \leq z_{\max} + \epsilon \quad \forall i \in W, \forall k \in T \quad (3.35)$$

$$\sum_{j \in T} x_{ijk} \leq 1 \quad \forall i \in W, \forall k \in T \quad \text{for } k = 0 \quad (3.36)$$

$$\sum_{j \in T} x_{ijk} \leq \sum_{j \in T} x_{ijk-1} \quad \forall i \in W, \forall k \in T \quad \text{for } k > 0 \quad (3.37)$$

$$z_{i*k} \geq 0 \quad \forall i \in W, \forall k \in T \quad (3.38)$$

$$M = \max_a a_i + \max_p \sum_{i \in W} \sum_{j \in T} p_{ij} \quad (3.39)$$

$$\epsilon = 1 \times 10^{-4} \quad (3.40)$$

Table 3.1 shows the computational complexity for the methods outlined in this chapter. The MSA method is the simplest solver and exhibits a linear complexity compared to the DMF method

proposed by Zeng and Zhao. As it can be seen the methods implemented in this thesis, specifically the ESDMF method, both solves the DMF method and does it by keeping the same linear complexity as the MSA method. The ST method proposed in this thesis exhibits a higher computational complexity but achieves a better optimization. This trade-off however requires a more in depth explanation which will follow in Section 4.2.

Solver	Computation Costs
MSA	$O(mn)$
DMF	$O(mn^2)$
SDMF	$O(mn^2)$
ESDMF	$O(mn)$
ST	$O(m^2n^2)$

Table 3.1: Comparison of computational costs for different solvers

3.3 Reinforcement Learning Theory

In this section the RL approach used to solve the different role resolution problems is depicted. Initially a foundation basis in the required knowledge is depicted and afterwards the description of the analysis environment implementation is presented.

3.3.1 Reinforcement Learning Definition

RL is a novel approach originated as a branch from the broader field of machine learning. It is an automated approach to understanding and automating learning and decision-making [Sutton and Barto, 2017, p. 15]. It distinguishes itself from other approaches by its novel focus on learning thanks to an agent which directly interacts with its environment, without the necessity of relying on training sets [Sutton and Barto, 2017, p. 15].

The formal framework used by RL defines the interaction between the so called learning agent and its environment by means of states, actions and rewards [Sutton and Barto, 2017, p. 15].

Key concepts in the field of RL are those of values and value functions which helps distinguish RL methods from evolutionary methods which have to undergo scalar evaluations of entire policies [Sutton and Barto, 2017, p. 15].

3.3.2 Finite Markov Decision Processes

RL approaches learn by interacting with the environment in order to achieve a goal. The agent interacting with the environment does this in a sequence of discrete time steps, it performs actions (choices made by the agent), reaches then states (basis for making decisions) and eventually receives rewards (basis for evaluating the choices) [Sutton and Barto, 2017, p. 73]. Moreover, a policy is a stochastic rule that the agent relies upon to choose actions as a function of states [Sutton and Barto, 2017, p. 73]. Ultimately, the sole goal of the agent is to maximize the reward that it receives over time [Sutton and Barto, 2017, p. 73].

Returns are modeled as functions of future rewards that an agents must maximize [Sutton and Barto, 2017, p. 73]. There exist two types of return functions which depend on the nature of the tasks and a discounting preference: 1. for episodic tasks a non discontinued approach is preferred

while 2. for continuous tasks, however, a discounted approach is better suited [Sutton and Barto, 2017, p. 73].

Equation 3.41 defines the sum of the rewards received over time step t :

$$G_t \doteq R_{t+1} + R_{t+2} + R_{t+3} + \cdots R_T \quad (3.41)$$

If we account for discounting, Equation 3.41 has to be slightly adapted by introducing a discounting factor γ and can be found in Equation 3.42:

$$G_t \doteq R_{t+1} + R_{t+2} + R_{t+3} + \cdots = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \quad (3.42)$$

where $0 \leq \gamma \leq 1$.

An environment with which one agent interacts, can satisfy a Markov property if the information contained at present effectively summarizes the past without affecting the capability of effectively predicting the future [Sutton and Barto, 2017, p. 73]. If the Markov property is satisfied, then this environment is called a MDP [Sutton and Barto, 2017, p. 73].

Last but not least, value functions are used to assign each state or state-action pair an expected return based on the policy used by the agent [Sutton and Barto, 2017, p. 74]. Optimal value functions assign the highest achievable return by any policy to a state or state-action pair and such policies, whose values are optimal, are called optimal policies [Sutton and Barto, 2017, p. 74].

Optimal state-value functions v_* are formally defined as follows:

$$v_*(s) \doteq \max_{\pi} v_{\pi}(s) \quad (3.43)$$

whereas optimal AV functions q_* are formally defined as follows:

$$q_*(s, a) \doteq \max_{\pi} q_{\pi}(s, a) \quad (3.44)$$

3.3.3 Dynamic Programming

Dynamic programming (DP) is a set of ideas and algorithms that can be used to solve MDPs [Sutton and Barto, 2017, p. 95]. There are two approaches in dynamic programming for solving MDPs: 1. policy evaluations is the iterative computation of value functions of a given policy and 2. policy improvement is the idea of computing an improved policy under the conditions of its given value functions [Sutton and Barto, 2017, p. 95].

By combining these two approaches we obtain the two most notable DP methods *i.e.*, policy and value iteration [Sutton and Barto, 2017, p. 95].

One captivating property of DP methods is the concept of bootstrapping: updating estimates of values of states by approximating the values of future states [Sutton and Barto, 2017, p. 96].

3.3.4 Monte Carlo Methods

MC methods use experience in form of sample episodes in order to learn value functions and optimal policies [Sutton and Barto, 2017, p. 123]. This approach yields different advantages over the DP methods seen in Subsection 3.3.3: 1. they do not need a model of the environment's dynamics as they learn the optimal solutions by merely interacting with the environment, 2. since they learn from sample episodes, they are very well suited for simulation environments, 3. it is efficient and surprisingly easy to use MC methods to focus on smaller regions or subsets of a problem and

4. MC methods are more robust when it comes to violations of the Markov property since they do not bootstrap for updating their values [Sutton and Barto, 2017, p. 123].

One of the drawbacks that MC methods bring along is the concept of maintaining sufficient exploration: by always acting greedily, alternative states will never yield their returns thus potentially never learning that they might prove to be better [Sutton and Barto, 2017, p. 123].

A MC simplified method can be formally defined as follows:

$$V(S_t) \leftarrow V(S_t) + \alpha[G_t - V(S_t)] \quad (3.45)$$

where G_t is the discounted return function defined by Equation 3.42 and α is a constant step-size parameter [Sutton and Barto, 2017, p. 127]. MC methods must wait until the end of one episode in order to evaluate the incremental value of $V(S_t)$ since only at that point in time G_t is known [Sutton and Barto, 2017, p. 128].

3.3.5 Temporal Difference Learning

TD are yet another set of learning methods for RL. Compared to the MC methods explained in Subsection 3.3.4, TD methods do not need to wait all the way up to the end of an episode to actually learn, they only must wait until the next step *i.e.*, they can bootstrap [Sutton and Barto, 2017, p. 128]. When they reach time step $t + 1$, they observe a reward R_{t+1} which then use to estimate $V(S_{t+1})$ [Sutton and Barto, 2017, p. 128]. The simplest TD method, which is called $TD(0)$, is defined as follows:

$$V(S_t) \leftarrow V(S_t) + \alpha[R_{t+1} + \gamma V(S_{t+1}) - V(S_t)] \quad (3.46)$$

TD methods, same as MC methods, are not excluded from the sufficient exploration methods [Sutton and Barto, 2017, p. 147]. TD methods deal with this complication in two different ways: 1. ONP by using an algorithm called State-Action-Reward-State-Action (SARSA) and 2. OP by using an algorithm called Q-learning [Sutton and Barto, 2017, p. 128].

3.3.6 On Policy Prediction with Approximation

Up until now, the different methods presented are not suited for arbitrarily large state spaces. However, there exist solution to tackle such large state spaces: approximate solution methods. Under the assumption that one must always account for finite and limited computational resources, it is not feasible to find an optimal policy or value function, instead we have to settle for a good approximation of the solution [Sutton and Barto, 2017, p. 189].

An essential characteristic for RL algorithms venturing in the area of approximation is being able of generalization *i.e.*, using experience from a limited subset of the state space to effectively generalize and produce a valid approximation of a much larger subset [Sutton and Barto, 2017, p. 189]. RL methods are capable of achieving this by relying on supervised-learning function approximation which essentially use backups as training example [Sutton and Barto, 2017, p. 222]. Specifically, one brilliant set of methods are those using parametrized function approximation *i.e.*, the policy is parametrized by a weight vector θ .

The parametrized functional form with weight vector θ can be used to write $\hat{v}(s, \theta) \approx v_\pi(s)$, which is the approximated value of state s given weight vector θ [Sutton and Barto, 2017, p. 191].

It is then clear that the weight vector θ has to be chosen wisely: this can be done by using variations of Stochastic Gradient Descent (SGD) methods [Sutton and Barto, 2017, p. 223]. SGD methods adjust the weight vector after each step by a tiny amount following the direction that would reduce the error the most:

$$\theta_{t+1} \doteq \theta_t - \frac{1}{2} \alpha \nabla [v_\pi(S_t) - \hat{v}(S_t, \theta_t)]^2 \quad (3.47)$$

$$= \theta_t + \alpha [v_\pi(S_t) - \hat{v}(S_t, \theta_t)] \nabla \hat{v}(S_t, \theta_t) \quad (3.48)$$

where α is a positive step size parameter and $\nabla f(\theta)$:

$$\nabla f(\theta) \doteq \left(\frac{\partial f(\theta)}{\partial \theta_1}, \frac{\partial f(\theta)}{\partial \theta_2}, \dots, \frac{\partial f(\theta)}{\partial \theta_n} \right)^\top \quad (3.49)$$

is the vector of partial derivatives with respect to θ [Sutton and Barto, 2017, p. 195].

An exceptional case is linear methods for function approximation, where the approximate function $\hat{v}(\cdot, \theta)$ is a linear function of the weight vector θ [Sutton and Barto, 2017, p. 198]. This means that for each state s there is a corresponding vector of features $\phi(s) \doteq (\phi_1(s), \phi_2(s), \dots, \phi_n(s))^\top$ which has the same number of components as θ [Sutton and Barto, 2017, p. 198]. With this definition in mind, we can now formally define the state-VFA as the inner product between θ and $\phi(s)$:

$$\hat{v}(s, \theta) \doteq \theta^\top \phi(s) \doteq \sum_{i=1}^n \theta_i \phi_i(s) \quad (3.50)$$

This simplified case of linear function approximation for state-value functions finally brings us to how we can use the SGD:

$$\nabla \hat{v}(s, \theta) = \phi(s) \quad (3.51)$$

Equation 3.51 tells us that for the simple linear case the SGD is nothing more than the corresponding features value [Sutton and Barto, 2017, p. 199].

Artificial Neural Networks

Up to this point, we considered linear function approximation. ANNs can be used instead for nonlinear function approximation [Sutton and Barto, 2017, p. 199]. The simplest case of an ANNs is a single feedforward perceptron, meaning that it has only one hidden layer (*i.e.*, a layer that is neither an input nor an output layer) and that the ANNs at hand has no loops between its neurons, meaning that the output can not influence the input (compared to recurrent ANNs, in which the output indeed can influence the input) [Sutton and Barto, 2017, p. 216].

The connections between neurons inside an ANNs are called weights and the analogy to its human counterpart is how strong synaptic connections are [Sutton and Barto, 2017, p. 216]. Refer to Figure 3.7 for a depiction of a single layer ANNs.

The key about solving nonlinearity with ANNs is how they apply nonlinear functions to the sum of their weights, this process is done by means of activation functions [Sutton and Barto, 2017, p. 216]. There are different types of activation functions that can be used but each one of the usually exhibits an “S” shape (*i.e.*, sigmoid), such as the sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$, the $\tanh(x) = 2\sigma(2x) - 1$ or the different classes of ReLUs, which have become captivating in the last few years due to their peculiar characteristics such as $f(x) = \max(0, x)$ [Sutton and Barto, 2017, p. 216].

Even though single layer perceptrons are powerful enough to approximate nonlinearity, in the past years a development toward more complex ANNs with multiple hidden layers (*i.e.*, multi-layer perceptrons) has been on the rise [Sutton and Barto, 2017, p. 217]. These complex ANNs allow to solve many artificial intelligence tasks in a much more efficient way [Bengio, 2009]. This

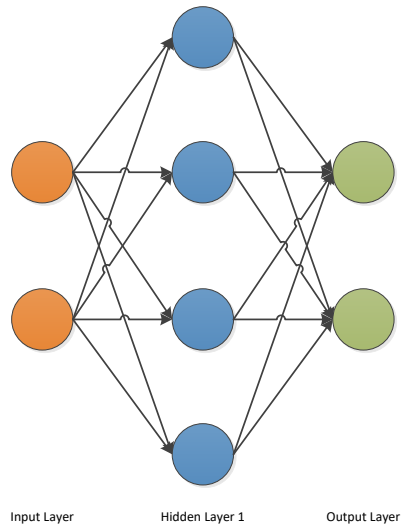


Figure 3.7: Single layer ANNs

area is called deep RL and it has shed light on solutions that were never though possible before (for practical applications refer to Mnih’s [Mnih et al., 2015] and Silver’s work [Silver et al., 2016])¹² [Bengio, 2009]. Refer to Figure 3.8 for a depiction of a multi layer ANNs.

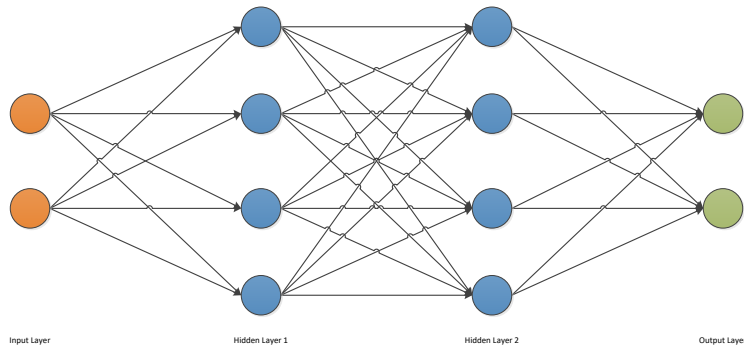


Figure 3.8: Multi layer ANNs

Despite appearing more complex, ANNs rely on a similar approach for learning (*i.e.*, updating their internal parameters, or in this case the whole network synaptic connections) based on the SGD method outlined in Subsection 3.3.6 [Sutton and Barto, 2017, p. 217]. This algorithm is called backpropagation and consists of doing a forward pass in which the activation function of

¹²Note that the class of deep ANNs used in these works is a particular one called deep convolutional networks, which are specialized networks used for processing high dimensional data arranged in spatial arrays like images [Sutton and Barto, 2017, p. 219], [Lecun et al., 1998].

each neuron is computed and then a backward pass computes the partial derivatives for each synaptic connection [Sutton and Barto, 2017, p. 218].

As any other function approximation method, overfitting can be a problem for ANNs as well and it is particularly present for deep ANNs [Sutton and Barto, 2017, p. 218]. There are different techniques that can be used in order to mitigate this effect, with the most prominent one being the dropout method outlined by Srivastava [Srivastava et al., 2014].

3.3.7 On Policy Control with Approximation

Moving towards control with VFA, we now focus on the approximation of the AV function $\hat{q}(s, a, \theta) \approx q_*(s, a)$ [Sutton and Barto, 2017, p. 229].

For the special case of the so called one-step SARSA method, its gradient-descent update for the AV function is defined as follows:

$$\theta_{t+1} \doteq \theta_t + \alpha [R_{t+1} + \gamma \hat{q}(S_{t+1}, A_{t+1}, \theta_t) - \hat{q}(S_t, A_t, \theta_t)] \nabla \hat{q}(S_t, A_t, \theta_t) \quad (3.52)$$

and this method has excellent good convergence properties towards optimality [Sutton and Barto, 2017, p. 230].

3.3.8 Off Policy Methods with Approximation

When moving towards the field of OP learning, one of the biggest problems that one might incur in is the convergence problem: OP learning with approximation is considerably harder compared to its tabular counterpart [Sutton and Barto, 2017, p. 243]. OP learning defines two policies, π and μ , where the former is the value function we seek to learn based on the latter [Sutton and Barto, 2017, p. 243].

A new aspect being introduced in OP learning is the importance sampling concept, formally defined as follow:

$$\rho_t \doteq \frac{\pi(A_t|S_t)}{\mu(A_t|S_t)} \quad (3.53)$$

which can be used to “warp the update distribution back to the ONP distribution, so that semi-gradient methods are guaranteed to converge.” [Sutton and Barto, 2017, p. 243].

During OP learning, both policies π and μ are usually defined as full greedy and somewhat more exploratory EP [Sutton and Barto, 2017, p. 243].

For the purpose of this thesis, the focus has been put upon the episodic AV update algorithms, defined as follows:

$$\theta_{t+1} \doteq \theta_t + \alpha \delta_t \nabla \hat{q}(S_t, A_t, \theta_t) \quad (3.54)$$

$$\delta_t \doteq R_{t+1} + \gamma \underbrace{\sum_a \pi(a|S_{t+1}) \hat{q}(S_{t+1}, a, \theta_t)}_{\max_a \hat{q}(S_{t+1}, a, \theta_t)} - \hat{q}(S_t, A_t, \theta_t) \quad (3.55)$$

what is important to note here, is that the episodic OP algorithm does not use importance sampling as defined by Equation 3.53 [Sutton and Barto, 2017, p. 244]. The authors state that this approach is clear for tabular methods but it is rather a “judgment call” for methods using approximation functions and deeper understanding of the theory of function approximation is needed [Sutton and Barto, 2017, p. 244].

3.3.9 Policy Gradient Methods

Up until now all methods were based on the concept of learning values of actions and subsequently choosing the correct actions based on estimates, however, we now move our focus towards methods that actually learn a parametrized policy without needing value functions at all¹³ [Sutton and Barto, 2017, p. 265]. Parametrized policies work with probabilities that a specific action a will be chosen at time t if the agent finds itself in state s at time t with a weight vector θ [Sutton and Barto, 2017, p. 265]. For PG methods it is crucial to learn the weight vector based on a performance measure $\eta(\theta)$ by trying to maximize and thus approximating the gradient ascent of η as follows:

$$\theta_{t+1} \doteq \theta_t + \alpha \widehat{\nabla \eta(\theta_t)} \quad (3.56)$$

where $\widehat{\nabla \eta(\theta_t)}$ is nothing else than a stochastic estimate that approximates the gradient of $\eta(\theta)$ [Sutton and Barto, 2017, p. 265].

For discrete action spaces, a suitable solution consists in forming parametrized numerical preferences $h(s, a, \theta) \in \mathbb{R}$ [Sutton and Barto, 2017, p. 266]. This means that the best actions is given the highest probability according to a softmax distribution:

$$\pi(a|s, \theta) \doteq \frac{e^{h(s, a, \theta)}}{\sum_b e^{h(s, b, \theta)}} \quad (3.57)$$

where $e \approx 2.71828$ [Sutton and Barto, 2017, p. 266].

Moreover, the preferences can be, as previously mentioned:

$$h(s, a, \theta) \doteq \theta^\top \phi(s, a) \quad (3.58)$$

i.e., simply linear in features [Sutton and Barto, 2017, p. 266].

With these definitions in mind, one can formally define one of the very first MC based PG methods: REINFORCE [Williams, 1992].

Williams defines his REINFORCE algorithm by the following update function:

$$\theta_{t+1} \doteq \theta_t + \alpha \gamma^t G_t \frac{\nabla_\theta \pi(A_t|S_t, \theta)}{\pi(A_t|S_t, \theta)} \quad (3.59)$$

note that the vector $\frac{\nabla_\theta \pi(A_t|S_t, \theta)}{\pi(A_t|S_t, \theta)}$ is called eligibility vector and it is usually written in a more compact form of $\nabla \log \pi(A_t|S_t, \theta)$ by relying on the mathematical identity $\nabla \log x = \frac{\nabla x}{x}$ [Sutton and Barto, 2017, p. 271].

For the REINFORCE algorithm, its eligibility vector is defined as follows:

$$\nabla_\theta \log \pi(a|s, \theta) = \phi(s, a) - \sum_b \pi(b|s, \theta) \phi(s, b) \quad (3.60)$$

and this method has solid convergence properties [Sutton and Barto, 2017, p. 271].

Policy Gradient with Baseline

REINFORCE, however, being a method based on MC it might exhibit high variance and prove relatively slow in its learning rate [Sutton and Barto, 2017, p. 271]. By introducing a baseline $b(s)$ to compare the AV:

¹³AC methods are an exception, where a learned value function is used in combination with PG as a baseline in order to lower variance.

$$\theta_{t+1} \doteq \theta_t + \alpha(G_t - \overbrace{b(S_t)}^{\text{baseline}}) \frac{\nabla_{\theta} \pi(A_t|S_t, \theta)}{\pi(A_t|S_t, \theta)} \quad (3.61)$$

one can achieve a positive effect towards diminishing variance of the update rule [Sutton and Barto, 2017, p. 271].

Actor Critic Policy Gradient

By introducing a base line, we have seen that variance can be lowered, however, the REINFORCE algorithm with a baseline is not a proper AC method as its state-value function is only used as baseline and not as a critic *i.e.*, it is not used for bootstrapping [Sutton and Barto, 2017, p. 273]. By introducing bootstrapping we introduce bias and dependence of the quality of the approximated function, which in turn help to reduce variance and learn faster [Sutton and Barto, 2017, p. 273].

The only negative aspect still remaining is that PG methods are still based on a full MC update trajectory: this can be also mitigated by replacing the update function by TD learning approaches, such as those defined in Subsection 3.3.5 [Sutton and Barto, 2017, p. 273].

The formal definition of a one-step AC update method is depicted as follows:

$$\theta_{t+1} \doteq \theta_t + \alpha(R_{t+1} + \overbrace{\gamma \hat{v}(S_{t+1}, w) - \hat{v}(S_t, w)}^{\text{TD update}}) \frac{\nabla_{\theta} \pi(A_t|S_t, \theta)}{\pi(A_t|S_t, \theta)} \quad (3.62)$$

and this is now a fully online implementation that executes updated after each newly visited state [Sutton and Barto, 2017, p. 274].

3.4 Reinforcement Learning Policies

Analog to Section 3.2, the same policies are considered where now different RL methods and techniques are used to solve the assignment problem.

Different subsections are used in order to separate better the different approaches used for each type of policy: 1. Batch policy methods. 2. LLQP policy methods. 3. other policy methods that do not fit in any of the previous categories.

The two key concepts required in order to effectively apply RL techniques in the domain of workflow processes and the optimal assignment of jobs to users are: 1. correctly defined states and actions spaces. 2. precise rewards definition. 3. effective update method for the policy's internal parameters.

In the next subsections a distinction between prediction and update methods is outlined.

3.4.1 Prediction and Control Methods

As previously outlined in Subsection 3.3.6, Subsection 3.3.7, Subsection 3.3.8 and Subsection 3.3.9 there are different prediction and control methods that can be applied.

Value Function Approximation

As mentioned in Section 3.4, it is crucial to correctly define the states and actions space for each problem. Each request that the policy receives generates a policy job object which is then passed in the internal evaluate method of the policy. Inside this method, for each policy job the state space S is defined as a $n \times n + 1$ matrix which contains all busy times of the potential candidates

(*i.e.*, users) concatenated to the user's current service time for the job. Formally the state space is defined as depicted in Equation 3.63:

$$S_{n,n+1} = \begin{bmatrix} a_1 & \cdots & a_1 \\ a_2 & \cdots & a_2 \\ \vdots & \ddots & \vdots \\ p_{1,j} & \cdots & p_{i,j} \end{bmatrix} \quad (3.63)$$

Since the possible actions are represented by the number of users, the state space is modeled such that for each possible actions a 1-D vector containing all busy times plus the service time of the user are present.

During the evaluation phase of a job the policy has to choose an action (*i.e.*, a user) by taking into account the current state space and its internal θ parameters. By using a state-VFA as defined in Equation 3.50, the policy evaluates the highest score for each possible user.

As an example, let us consider a snippet of how a K-Batch policy using a linear state-VFA performs its choices during its greedy phase: it iterates over all possible actions and performs the dot product between the state space and the corresponding θ vector and then maximizes the returned Q value. This approach can be seen in Listing 3.4

```
if self.greedy:
    action = max(range(self.number_of_users), key=lambda action: self.q(
        state_space, action))
else:
    rnd = self.EPSILON_GREEDY_RANDOM_STATE.rand()
    if rnd < self.epsilon:
        action = self.EPSILON_GREEDY_RANDOM_STATE.randint(0, self.
            number_of_users)
    else:
        action = max(range(self.number_of_users), key=lambda action: self.q(
            state_space, action))
```

Listing 3.4: EP approach

and its respective state-VFA in Listing 3.5.

```
def q(self, states, action):
    features = self.features(states, action)
    q = np.dot(features[action], self.theta[action])
    return q
```

Listing 3.5: State-VFA

Q values are however only one part of the requirements set by RL methods, the next crucial aspect is defining the reward function. Since RL agents are able to back-propagate what they have learned from one episode and thus update their internal factors, correctly defining a reward is a must. Since the goal for our domain is minimizing the maximum flowtime (from now on this metric will be referred to as lateness) of a job, the reward itself corresponds to the lateness of a job during a specific task. This can be evaluated a priori since for each policy job we know its internal parameters required to calculate the lateness *i.e.*, busy time of user i plus the service time of user i for job j , or formally $a_i + p_{ij}$.

The last definition required in order to effectively apply the update on the policy's internal parameters θ is defining the SGD method as outlined by Equation 3.51. This method will give us the direction in which we have to update our internal θ parameters during our chosen update

method and it is nothing more than the features themselves. As an example, refer to Listing 3.6 for the concrete implementation.

```
def features(self, states, action):
    features = np.zeros((self.number_of_users, self.number_of_users + 1))
    features[action] = states[action]
    return features
```

Listing 3.6: Features definition

The features method outputs a matrix which has its values populated only for the actual chosen action. Let us assume our policy has chosen user 1 out of 2 possible users, then the state space looks as defined by Equation 3.64:

$$S_{2,3} = \begin{bmatrix} a_1 & a_1 \\ a_2 & a_2 \\ p_{1,j} & p_{2,j} \end{bmatrix} \quad (3.64)$$

and its features vector looks as defined by Equation 3.65:

$$F_{2,3} = \begin{bmatrix} a_1 & 0 \\ a_2 & 0 \\ p_{1,j} & 0 \end{bmatrix} \quad (3.65)$$

Policy Gradient

With PG methods the approach on how an action is chosen is shifted. Instead of maximizing a Q value through internal θ parameters in order to choose the “best greedy” action, we now have probabilistic choices. As already outlined in Subsection 3.3.9, having a probabilistic policy π means that the best action is now chosen according to the highest probability which follows a softmax distribution as defined in Equation 3.57 and its implementation can be seen in Listing 3.7.

```
def policy_probabilities(self, busy_times):
    probabilities = [None] * self.number_of_users
    for action in range(self.number_of_users):
        probabilities[action] = np.exp(np.dot(self.features(busy_times, action),
            self.theta)) / sum(
                np.exp(np.dot(self.features(busy_times, a), self.theta)) for a in
                    range(self.number_of_users))
    return probabilities
```

Listing 3.7: Softmax distribution of preferences probabilities

The policy probabilities method takes as input parameter the current state space and computes for each user its probability according to the current internal θ parameter as defined in Equation 3.58. The result of this method is a probabilities (or weights) 1-D vector corresponding to a preference to assign a job to a specific user, where the index of the vector corresponds to the user and the value to its preference. Based on this preferences vector, the policy then computes a weighted random choice among all users, as can be seen in Listing 3.8.

```
chosen_action = self.RANDOM_STATE_PROBABILITIES.choice(self.number_of_users,
    p=probabilities)
```

Listing 3.8: Probabilistic user choice

Artificial Neural Networks as Function Approximation

Up to this point we have used linear functions for the approximation of the Q value for the different policies. As mentioned in Subsection 3.3.6, ANNs can be used for nonlinear function approximation. The assignment problem poses its very well for this kind of application, in which we model our input layer as a 1-D vector containing all required information such as waiting time w of job j , service time p_{ij} of user i for job j and busy time a_i of user i . By following a PG approach, we can categorize the output layer of our ANNs using a softmax categorization function, mapping the preferences of job j to user i assignment as probabilities. Listing 3.9 show the modeling of a single layer perceptron in TF: one hidden layer connects the state space (*i.e.*, input to the ANNs) together with its weights and biases, creates an activation function and maps the prediction layer (*i.e.*, output) with a softmax classification.

```
with tf.name_scope("neural_network"):
    layer_1 = tf.add(tf.matmul(state_space_input, weights['h1']), biases['b1'])
    layer_1 = tf.nn.elu(layer_1)
    pred = [tf.add(tf.matmul(layer_1, weights['out'])[b]), biases['out'][b]]
    for b in range(batch_input):
        probabilities = [tf.nn.softmax(pred[b]) for b in range(batch_input)]
```

Listing 3.9: Modeling of a single perceptron in TF

In order to update the ANNs, a backpropagation has to take place. Such an update can both be made following a MC or TD approach (refer to Subsection 3.4.2 for a detailed distinction between these two update methods). As outlined in Subsection 3.3.6, we follow a SGD approach in which we update all the synaptic connections by computing the partial derivatives of all the weights. Listing 3.10 shows how the backpropagation for an ANNs following a MC update method is done.

```
def train(self):
    for t, (state, output, choices) in enumerate(self.history):
        disc_rewards = self.discount_rewards(t)
        tmp_choices = [choice for choice in choices if choice is not None]
        for job_index, chosen_user in enumerate(tmp_choices):
            prob_value = output[job_index].flatten()[chosen_user]
            reward = disc_rewards[job_index]
            factor = reward / prob_value
            grad_input = np.zeros((self.number_of_users, 1))
            grad_input[chosen_user] = 1.0
            self.sess.run(self.apply[job_index], {self.state_space_input: state,
            self.gradient_input: grad_input, self.factor_input: factor})
```

Listing 3.10: Backpropagation algorithm following a MC update approach

3.4.2 Update Methods

As outlined in Subsection 3.3.4 and Subsection 3.3.5, there are mainly two different methods to update the policy's internal θ parameters *i.e.*, MC and TD. Let us take the example outlined by Sutton and Barto of leaving the office and getting home and the respective updates proposed by the two update methods [Sutton and Barto, 2017, p. 130]. Figure 3.9 shows the graphical updates proposed by the two update methods.

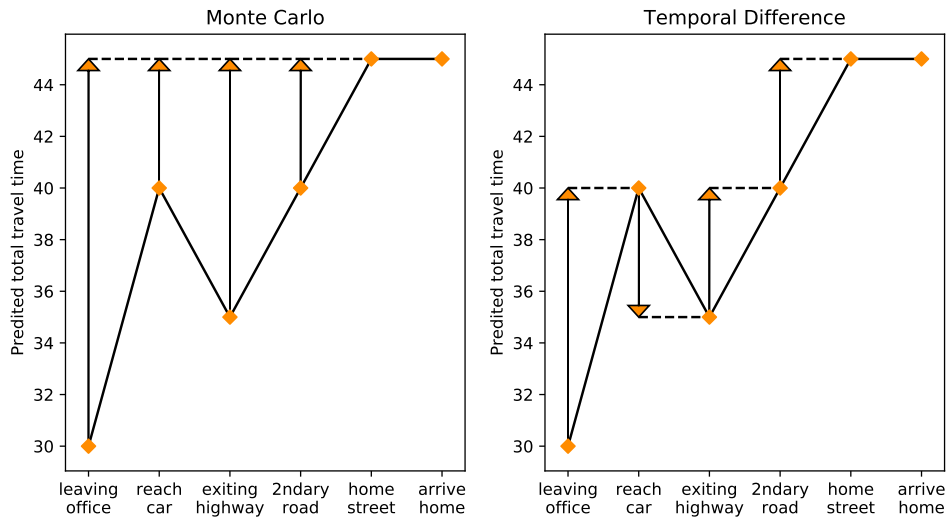


Figure 3.9: MC and TD proposed updates comparison (own plot based on [Sutton and Barto, 2017, p. 130])

As it can be clearly seen, the main difference lays in when the actual updating takes place. On one hand, the MC method needs to reach the end of an entire episode (*i.e.*, here it consists of actually arriving home) in order to fully back-propagate its learned value and update the θ parameters. On the other hand, TD is much more flexible and robust since it executes its updates at each time step, hence its name: TD. For a formal overview of the difference between the two update methods, refer to Equation 3.45 for the MC update and to Equation 3.46 for the TD update. For the case at hand, this means that training the policies has to be done in a different fashion for the two update methods: while TD based policies can be updated “on-the-fly”, MC methods require batch training sessions (*i.e.*, episodes) at the end of which they can effectively learn and update their internal θ parameters to be used for the next episode. Not only the training approach is different, but the logic of the policy itself is also different: for TD based policies, the update method is being called internally since the policy knows its temporal steps, while for MC based policies the policy itself can not know a priori when an episode will finish and thus must rely on an “artificial” definition of such. The overall overhead is also different since MC based policies have to keep track of their whole episode history which usually is composed of the state space, chosen action and reward at time step t .

Sutton and Barto outline a qualitative comparison between both update methods which can be found summarized in table Table 3.2.

Characteristic	MC	TD
Bootstrap	No	Yes
Update Time	End of episode	Each time step
Discount	Required	Not required
Convergence	Good	Very Good
Learning Rate	Slow for long episodes	Very fast even for long episodes

Table 3.2: Qualitative comparison between MC and TD update methods [Sutton and Barto, 2017, p. 130]

3.4.3 Batch Size Emulation

Correctly defined state spaces is a crucial requirement for effective RL methods. LLQP policies are relatively easy to be modeled, on the other hand policies with batch sizes require a more meticulous consideration. By introducing a batch size that retains jobs in its global queue (*i.e.*, all batch sizes $K > 1$), not only the job-to-user assignment plays a role, but the ordering of the assignment influences greatly the final outcome as well. Let us consider a simple case with users $i = 2$ and jobs $j = 3$ at time step t . Table 3.3 summarizes the service times p_{ij} in time units t of both users for all three jobs.

User	Job 1	Job 2	Job 3
User 1	1	2	3
User 2	4	5	6

Table 3.3: Service times of both users for all three jobs

It is clear that the ordering of the jobs assigned has an impact on the final outcome. Figure 3.10 outlines a possible conformation where user 1 receives job 1 while user 2 gets assigned to jobs 2 and 3 respectively. In this case, job 1 is started at t and is finished at $t + 1$, job 2 is started at t and is finished at $t + 5$ and job 3 is started at $t + 5$ and is finished at $t + 11$. The respective lateness per job is: 1 for job 1, 5 for job 2 and 6 for job 3.

By changing the assignment order (refer to Figure 3.11 for a graphical representation), the final outcome changes as well: In this case, job 1 is started at $t + 2$ and is finished at $t + 3$, job 2 is started at t and is finished at $t + 2$ and job 3 is started at t and is finished at $t + 6$. The respective lateness per job is: 1 for job 1, 2 for job 2 and 6 for job 3. By merely changing the assignment order a reduction of 40% in lateness is observed by job 2.

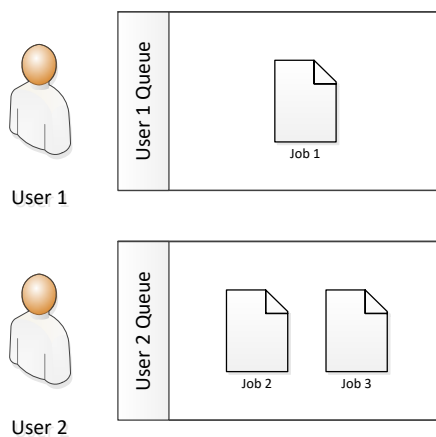


Figure 3.10: User 1 receives job 1 while user 2 receives jobs 2 and 3

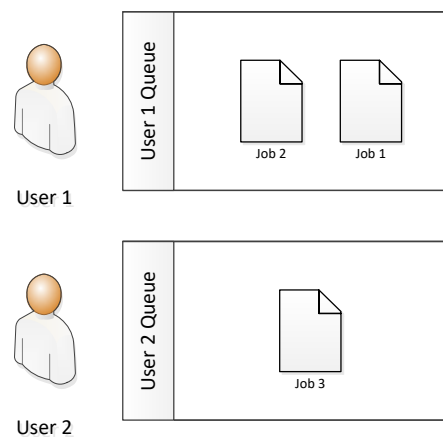


Figure 3.11: User 1 receives jobs 2 and 1 while user 2 receives job 3

Subsection 4.3.3 outlines three different types of policies (refer to Table 4.9 for a detailed explanation of the policies) that take into account the previously outlined job assignment ordering principle and exploit it in their state space modeling. This is done by means of integrating an additional parameter B that defines how many jobs have to be considered when trying to optimally assign jobs lying in the global queue to users. This is done by listing all possible combinations by accounting for the job order as well. Refer to Listing 3.11 for the actual implementation.

```
combinations = list(itertools.product(range(self.number_of_users), repeat=
    self.wait_size))
for i, combination in enumerate(combinations):
    state_space[i] = a + [p[user_index][job_index] for job_index, user_index
        in enumerate(combination)]
```

Listing 3.11: State space modeling by considering B jobs from the global queue and integrating all possible combinations

This approach effectively simulates batch policies with batch sizes $K > 1$.

Empirical Analysis

4.1 Methodology

In order to consistently and fairly evaluate all policies with the methods defined in the previous chapters, the following methodology was put in place: 1. Each policy has its own simulation script that initialized a process that uses the predefined policy as means to optimally assign jobs to tasks 2. Parameters are centrally defined. 3. Different KPIs have been defined which are used to assert the efficiency of one policy against one another.

4.1.1 Simulation script

Each simulation script is the abstract element that import all required dependencies, initializes the SimPy simulation environment, the statistics file into which the policy dumps all data on runtime, the policy object itself to be used for the assignment and the workflow process to be used.

```
import simpy
from evaluation.statistics import calculate_statistics
from evaluation.subplot_evolution import evolution
from policies.optimization.batch.k_batch import K_BATCH
from simulations import *
from solvers.dmf_solver import dmf

policy_name = "{}_BATCH_DMF_NU{}_GI{}_SIM{}".format(BATCH_SIZE,
    NUMBER_OF_USERS, GENERATION_INTERVAL, SEED, SIM_TIME)

env = simpy.Environment()

file_policy = create_files("{}_csv".format(policy_name))

policy = K_BATCH(env, NUMBER_OF_USERS, WORKER_VARIABILITY, file_policy,
    BATCH_SIZE, dmf)

start_event = acquisition_process(env, policy, 1, GENERATION_INTERVAL, False,
    None, None, None)

env.process(start_event.generate_tokens())
```

```

env.run(until=SIM_TIME)

file_policy.close()

calculate_statistics(file_policy.name, outfile=True)

evolution(file_policy.name, outfile=True)

```

Listing 4.1: Example of the structure of a simulation script. Here for the K-Batch policy using the DMF solver

The script initialized the chosen workflow process and then calls the tokens generation method of the start event. Eventually the whole simulation is started by calling the run method of the SimPy environment.

4.1.2 Workflow Process Modeling

Two different types of processes have been defined: 1. Consisting of only one user task. 2. A complex workflow process that is modeled against an acquisition process used in the real estate field for the acquisition of real estate properties.

Figure 4.1 illustrates the simple process.

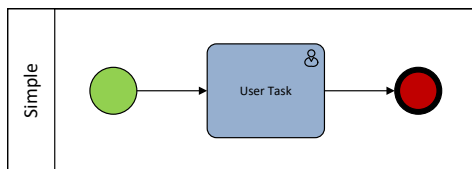


Figure 4.1: Simple workflow process consisting of only one user task

Figure 4.2 illustrates the complex acquisition process.

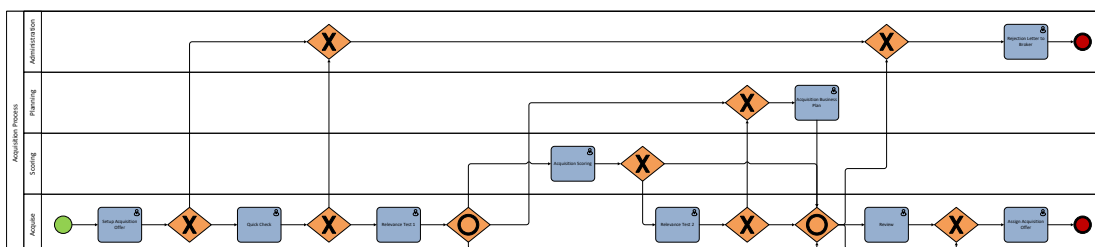


Figure 4.2: Acquisition workflow process consisting of multiple user tasks and decision nodes

4.1.3 Central Simulation and Process Parameters Definition

One key aspect in order to assert fairness across policies while simulated is to centrally define all parameters. Listing 4.2 shows the key central parameters defined as global variables.

```
NUMBER_OF_USERS = 3
SERVICE_INTERVAL = 1
GENERATION_INTERVAL = 3
SIM_TIME = 1000
BATCH_SIZE = 5
TASK_VARIABILITY = 0.2 * SERVICE_INTERVAL
WORKER_VARIABILITY = 0.2 * SERVICE_INTERVAL
SEED = 2
```

Listing 4.2: Central parameters definition that ensures fairness across simulation runs

4.1.4 KPIs for Asserting Policy's Efficacy and Data Visualization

Based on Pinedo's and Zeng and Zhao's definitions in their works, different KPIs have been defined to assert the efficacy of a policy, such as lateness, waiting time, service time, number of tokens completed, user loads and system load [Pinedo, 2008, Zeng and Zhao, 2005]. Following the formal definitions of the per token j KPIs in respect to lateness L_j , wait time w_j , service time p_{ij} of assigned user i , arrival time A_j , assignment time a_j , start time S_j and finish time F_j .

$$L_j = F_j - A_j \quad (4.1)$$

$$w_j = S_j - A_j \quad (4.2)$$

$$p_{ij} = F_j - S_j \quad (4.3)$$

Moreover, if we account for simulation time T , load l_i of user i is defined as the sum of all service times of tokens that have been assigned to him during the simulation divided by the total simulation time T , or formally:

$$l_i = \frac{\sum_j p_{ij}}{T} \quad (4.4)$$

and thus the average system load \bar{l} over all users participating n is defined as the average across all user's loads *i.e.*,

$$\bar{l} = \frac{\sum_i l_i}{n} \quad (4.5)$$

A summary plot with all KPIs is done for each simulation script. Figure 4.3 shows an example of how this summary looks like.

Additionally, for a more in depth visualization of a policy's performance, an evolution plot is also necessary. All types of policies share a common queues configuration, with a single global queue and a user specific queue. Each policy defines the maximal threshold a specific queue can reach. For a detailed explanation of the queues conformation refer to Section 3.2.

The evolution plot shows the state change for the policy being analyzed by plotting the flow of a token across different user tasks. Figure 4.4 shows such an example.

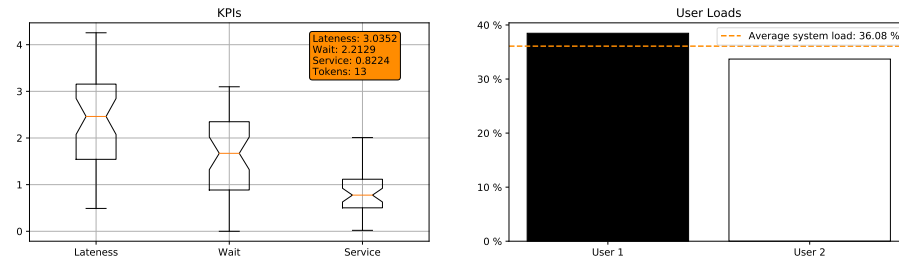


Figure 4.3: KPIs summary plot for a 3-Batch policy using the MSA solver, with two users, generation interval set to three and simulation time T set to 50

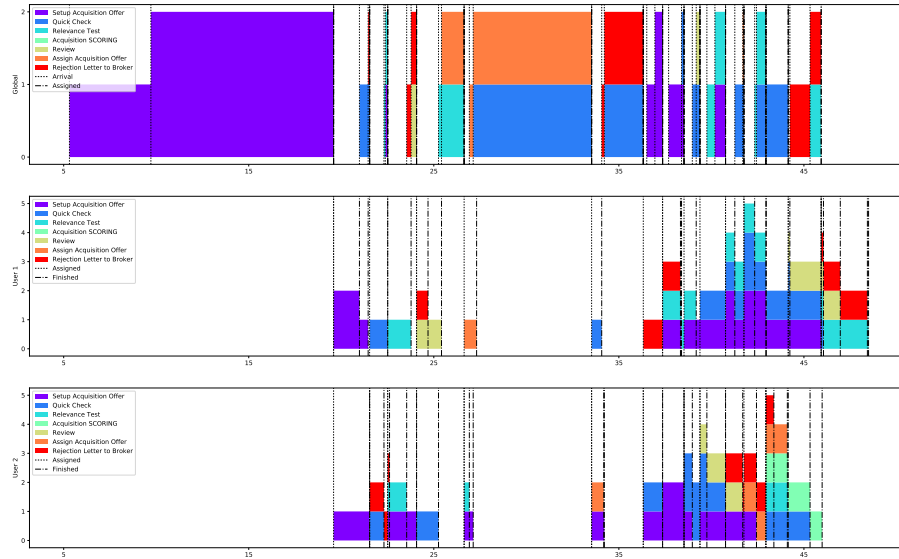


Figure 4.4: Evolution plot for a 3-Batch policy using the MSA solver, with two users, generation interval set to three and simulation time T set to 50

4.2 Optimization

This section focuses on the results of the different types of policies using the optimization solvers outlined in Section 3.2. All simulations have been tested with different combination of global variables *i.e.*, number of users, service interval, generation interval, length of simulation time, batch size (where it applies), task variability, worker variability and random state seed (where it applies). For ease of reading purposes, the global variables have been set to the following parameters according to the default column in Table 4.1.

Variable	Default	Valid Range
Number of Users	3	$1 - \infty$
Service Interval	1	$1 - \infty$
Generation Interval	3	$1 - \infty$
Simulation Time	1000	$1 - \infty$
Batch Size	5 (1 for 1-Batch-1)	$1 - \infty$
Task Variability	20%	$0\% - 100\%$
Worker Variability	20%	$0\% - 100\%$
Random State Seed	2	$\emptyset - \infty$
Workflow Process	Acquisition	Acquisition, Simple

Table 4.1: Global Parameters for Simulation

4.2.1 Comparison with Existing Literature

Zeng and Zhao outline in their work how different global parameters configurations and policy usage can affect KPIs [Zeng and Zhao, 2005, pp. 18-22]. They summarize their key findings as follows: 1. Usage of batch optimization should be done only with medium to high system load [Zeng and Zhao, 2005, p. 24]. 2. Batch optimization policies without a fixed batch size, such as 1-Batch-1 yield best results [Zeng and Zhao, 2005, p. 24].

In order to assert the validity of the interpretation of Zeng and Zhao's works and all subsequent derivative policies a comparison with similar configurations has been made for all five optimization policies. Zeng and Zhao's main efficiency parameter is defined as the maximum flowtime or in their own words: "In business terms, maximum flowtime represents the guaranteed response time across tasks, indicating the quality of services" [Zeng and Zhao, 2005, p. 17]. In this study, the comparable parameter used to evaluate a policy's efficiency is called lateness and has been previously defined in Equation 4.1. In regards to lateness, Figure 4.5 shows that akin results to Zeng and Zhao's are obtained.

The simulations have been run with the parameters outlined in Table 4.1 by using the same solver used by Zeng and Zhao: MSA.

By running the same simulations with the optimization solver implemented for this thesis (*i.e.*, ST, refer to Section 3.2), *ceteris paribus*, the summarized KPIs amongst all optimization policies can be seen in Figure 4.6.

The percent reduction for both batch policies with a higher batch size is tiny, but when considering the reduction between the 1-Batch-1 policy with MSA and ST, a wealthy reduction is present for all KPIs. For a detailed overview of the overall reductions of the ST against the MSA solver refer to Figure 4.7.

Astonishing reductions have been observed for the 1-Batch-1 policy, which is indeed the most

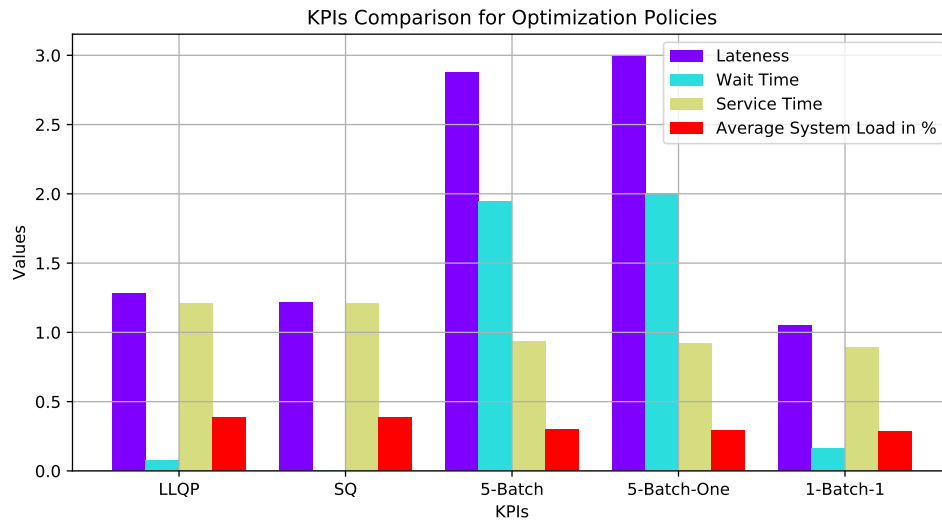


Figure 4.5: KPIs comparison for different optimization policies using the MSA solver for batch policies

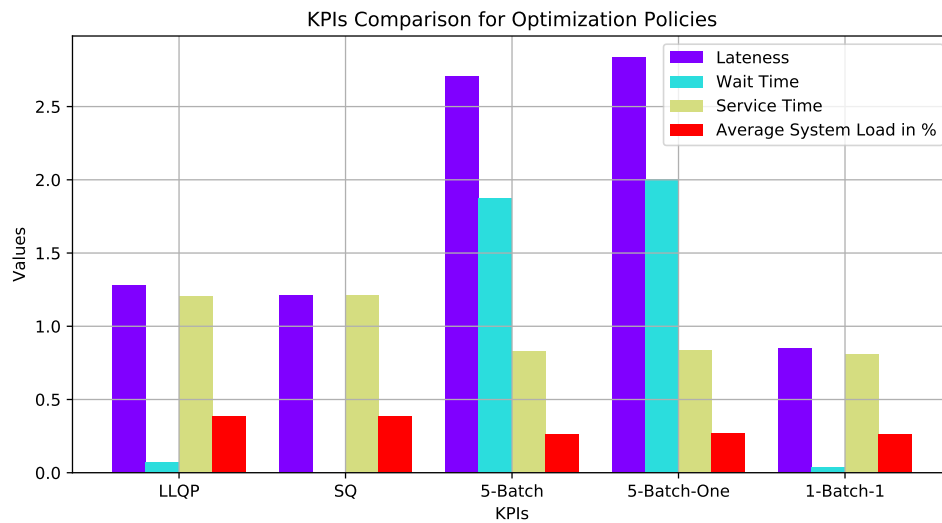


Figure 4.6: KPIs comparison for different optimization policies using the ST solver for batch policies

efficient policy as mentioned by Zeng and Zhao (for a detailed comparison of how different batch sizes affect the policy's KPIs refer to Subsection B.3.3 and Subsection B.4.3) [Zeng and Zhao, 2005, p. 24]. Table 4.2 summarizes these values.

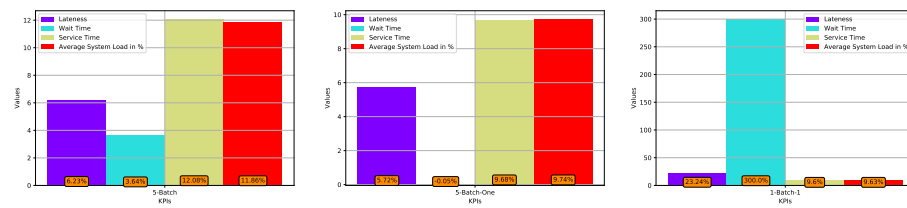


Figure 4.7: KPIs reduction comparison between the MSA and the ST solvers for different batch policies

KPI	Reduction (in %)
Lateness	23.24
Wait Time	300.0
Service Time	9.6
Average System Load	9.63

Table 4.2: Reduction (in %) across all KPIs of the ST against the MSA solver

4.3 Reinforcement Learning

This section focuses on the results obtained with the RL methods outlined in Section 3.4. A more in-depth review of the different policies is required, thus a finer subdivision has been made in different subsections per policy type: Subsection 4.3.1 focuses on batch policies, Subsection 4.3.2 focuses on LLQP policies and Subsection 4.3.3 focuses on all remaining policies that do not fit in either of the previous categories.

In order to maintain fairness amongst RL training methods, all required parameters are globally set and equal across all simulation scripts and can be found summarized in Table 4.3.

Parameter	Value
γ	0.5
α	0.0001
ϵ	0.1
MC epochs	1000
TD training time	1000

Table 4.3: Global RL parameters

Comparisons will be made, where not otherwise stated, with the corresponding optimization policy simulated under the same conditions.

4.3.1 Batch

Five different batch policies with RL have been developed. Table 4.4 gives an overview.

Technical Name	Policy Type	Update Method	Q Value Method	Other Characteristics
k_batch_mc_vfa	1-Batch	MC	VFA	None
k_batch_mc_vfa_op	1-Batch	MC	VFA	OP
k_batch_mc_vfa_o pep	1-Batch	MC	VFA	EP, OP
k_batch_td_vfa_op	1-Batch	TD	VFA	OP
k_batchone_td_vfa_op	1-Batch-1	TD	VFA	OP

Table 4.4: Overview of developed batch policies with RL

Table 4.5 shows the summarized results. For the detailed results refer to Subsection C.1.3 for 1-Batch respectively to Subsection C.2.3 for 1-Batch-1.

glskpi	k_batch_mc_vfa	k_batch_mc_vfa_op	k_batch_mc_vfa_o pep	k_batch_td_vfa_op	k_batchone_td_vfa_op
Lateness	32.96	33.88	32.75	33.71	20.33
Wait Time	230.3	226.58	167.28	248.98	44.4
Service Time	12.07	13.06	14.71	12.11	14.14
Average System Load	11.74	12.75	14.4	11.8	13.81

Table 4.5: Reduction (in %) across all KPIs of the batch policies with RL against the MSA solver

4.3.2 Least Loaded Qualified Person

Three different LLQP policies with RL have been developed. Table 4.6 gives an overview. Other policies have been implemented for evaluating different RL methods, however they are not considered for the final evaluation. These policies can be seen in Table C.1.

Technical Name	Policy Type	Update Method	Q Value Method	Other Characteristics
llqp_mc_vfa_op	LLQP	MC	VFA	OP
llqp_td_vfa_op	LLQP	TD	VFA	OP
llqp_td_tf_op	LLQP	TD	ANNs	OP

Table 4.6: Overview of developed LLQP policies with RL

Table 4.7 shows the summarized results. For the detailed results refer to Subsection C.3.3.

KPI	llqp_mc_vfa_op	llqp_td_vfa_op	llqp_td_tf_op
Lateness	0.18	0.21	0.81
Wait Time	2.98	0.81	10.8
Service Time	−0.14	0.14	−0.3
Average System Load	−0.15	0.19	−0.3

Table 4.7: Reduction (in %) across all KPIs of the LLQP policies with RL against the MSA solver

Table 4.8 shows the comparison between OP and ONP approaches.

KPI	llqp_mc_vfa_op	llqp_mc_vfa	difference (in %)
Lateness	1.3138	1.3422	−2.12
Wait Time	0.0874	0.1408	−37.93
Service Time	1.2264	1.2014	2.08
Average System Load	39.24%	38.49%	2.19

Table 4.8: KPIs comparison between OP and ONP approaches

4.3.3 Others

Three different additional policies with RL have been developed which have been used to fully emulate the behavior of K-Batch and 1-Batch-1 (as explained in Subsection 3.4.3). Table 4.9 gives an overview.

Table 4.10 shows the summarized results. For the detailed results refer to Subsection C.4.3.

Technical Name	Policy Type	Update Method	Q Value Method	Other Characteristics
wz_td_vfa_op	WZ	TD	VFA	OP
wz_one_td_vfa_op	WZO	TD	VFA	OP
bi_one_mc_tf	BI	MC	ANNs	PG

Table 4.9: Overview of additional developed policies with RL

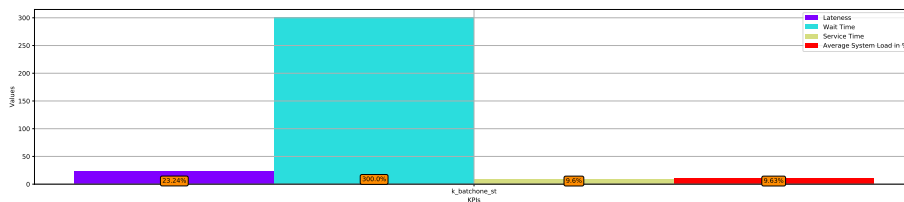
KPI	wz_td_vfa_op	wz_one_td_vfa_op	bi_one_mc_tf_1l	bi_one_mc_tf_2l	bi_one_mc_tf_3l	bi_one_mc_tf_4l
Lateness	-6.02	24.16	8.98	-12.12	-21.37	-18.8
Wait Time	-17.52	77.88	134.96	1.88	-28.06	-19.39
Service Time	20.76	13.08	-7.18	-15.87	-18.92	-18.6
Average System Load	20.58	12.76	-7.45	-15.95	-18.99	-18.68

Table 4.10: Reduction (in %) across all KPIs of the additional policies with RL against the MSA solver

4.4 Discussion

4.4.1 Optimization

Using mathematical optimization to solve the assignment problem proves to be an efficient measure, however different solvers yield different solutions and computational complexities. Zeng and Zhao mention that MSA greatly simplifies DMF since only those tasks that are immediately available are considered [Zeng and Zhao, 2005, p. 15]. This consideration is done since the DMF problem proves to be computationally expensive to solve [Zeng and Zhao, 2005, p. 13], [Garey and Johnson, 1990]. Zeng and Zhao propose however that by introducing auxiliary variables one can reduce the complexity of DMF and effectively solving it [Zeng and Zhao, 2005, p. 13]. This is what has been done in this thesis, as outlined in Section 3.2 by introducing new types of solvers. The ST “flagship” solver significantly outperforms the MSA solver (refer to Figure 4.8). Having said that, the higher computational complexity of ST compared to MSA (see Table 3.1) questions the practical use of this solver over the other methods. A 20% gain in respect to lateness requiring a quadratic higher computational complexity poses a dubious trade-off from a business perspective.

**Figure 4.8:** KPIs comparison between MSA and ST under 1-Batch-1

Yet another aspect mentioned by Zeng and Zhao is a more “social” aspect: the fairness of a policy *i.e.*, how fairly are single users treated by a policy during job assignment [Zeng and Zhao, 2005, pp. 17-18]. Figure 4.9 and Figure 4.10 both show how fairly are users treated in the same scenario by the two solvers.

It is clear that ST is “fairer” at balancing loads across users compared to MSA.

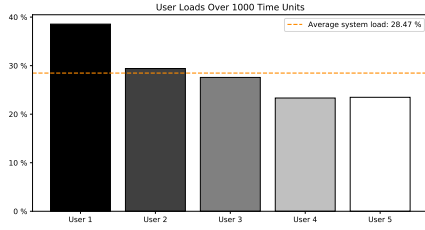


Figure 4.9: User loads distribution for 1-Batch-1 using MSA

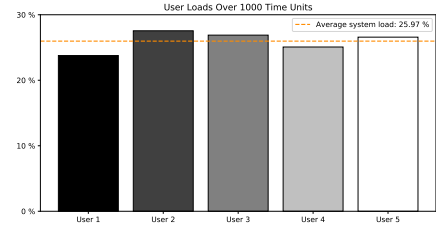


Figure 4.10: User loads distribution for 1-Batch-1 using ST

4.4.2 Reinforcement Learning

Let us first focus on LLQP, which, as explained in Section 3.2, focuses on assigning a job to the least loaded qualified person. By comparing the results obtained with RL against the optimization method, we clearly see that gains across all KPIs are imperceptible (refer to Subsection C.3.3 for more details). This sheds light on two key aspects: 1. LLQP policies are intrinsically optimized by their nature of implementation. 2. RL methods converge really well (for a 1000 time steps LLQP simulation, LLQP with TD and TF only needs 20 times the simulation time as training in order to perfectly converge to actual LLQP) and, even if only slightly, exploit internal mechanisms of LLQP policies to extract better results.

On the other hand, batch policies exhibit a much bigger optimization potential for which RL methods do really adapt well. Lateness improvements in the range of 30% for 1-Batch (see Subsection C.1.3) respectively 20% for 1-Batch-1 (see Subsection C.2.3) confirm the previous claim.

Lastly, when accounting for job order during assignment (refer to Subsection 3.4.3 for the detailed explanation), improvements are observed only under specific conditions: 1. by using WZO (see Figure C.24) and 2. ANNs with 1L (see Figure C.25).

Having said that, deep ANNs exhibits worse results compared to their equivalent emulated optimization methods. This can be explained from a twofold perspective: 1. VGP and 2. EGP.

In brief, VGP states that even very large change in partial derivatives on initial layers have imperceptible effects on subsequent layers [Bengio et al., 1994] and EGP states that huge spikes in the norm of changes in partial derivatives which could potentially grow exponentially can happen under training, thus influencing internal parameters [Bengio et al., 1994, Pascanu et al., 2012].

Yet another crucial aspect to consider when undergoing RL methods is usage between ONP or OP learning (refer to Subsection 3.3.6 and Subsection 3.3.7 for ONP respectively Subsection 3.3.8 for OP). As shown in Table 4.8 (and Figure 4.11), OP methods converge slightly better compared to ONP, however the change is imperceptible and can be found in different factors (*e.g.*, random state seed choice or length of simulation). Having said that, it is important to note that these different approaches are being currently heavily studied by pioneers and the debate is still open, as Sutton and Barto explain in their book [Sutton and Barto, 2017, pp. 245-249]. The current key takeaways from this outgoing debate can be summarized as follows [Sutton and Barto, 2017]: 1. Learning OP 2. Usage of scalable function approximation methods like linear semi-gradient 3. Usage of bootstrapping which is used in TD methods.

The combination of all these three factors is referred as “the deadly triad” [Sutton and Barto, 2017, p. 249]. Sutton and Barto argue that dangers can arise only when all three aspects are present, if used singularly convergence properties are safe [Sutton and Barto, 2017, p. 249].

On a more general note, different comparisons have shown huge spikes in reduction of wait-

ing time (e.g., Subsection C.1.3). Even though compelling, the practical usage is limited: when considering workflow processes with fixed available resources (*i.e.*, users participating), huge reduction in job waiting times does not always correlate with better system performance, since it might be the case that even if a job is ready to be assigned there are no available resources to complete such job.

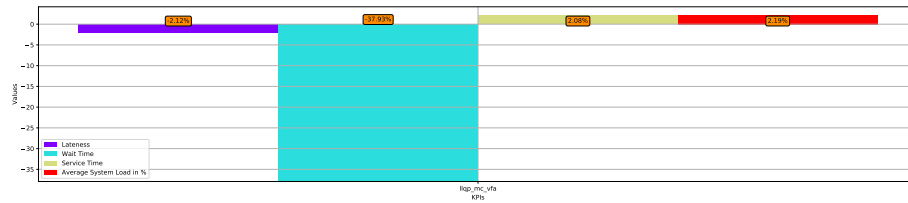


Figure 4.11: KPIs comparison between OP and ONP approaches

Conclusion

5.1 Summary

The focus of this thesis was analyzing different approaches for optimally allocating resources inside workflow processes by means of different methods.

Initially a found literature review has been made in order to establish the existing optimization solution (*i.e.*, foundations set by Zeng and Zhao [Zeng and Zhao, 2005]), then a roadmap on how to further develop such methods has been laid out. The roadmap encloses a two fold approach:

Appr. 1 Further develop mathematical optimizations

Appr. 2 Use RL methods as novel solution for optimal job assignment.

Subsequently, a discrete event simulation environment as outlined in Subsection 3.1.2 has been implemented which served as foundation for evaluating all future optimization policies.

For Approach 1 five existing optimization policies as outlined in Section 3.2 have been implemented and evaluated against the existing policies defined by Zeng and Zhao [Zeng and Zhao, 2005, pp. 13-14]. Furthermore, for Approach 2 a profound literature review about RL had to be made and following on the theoretical foundations laid (see Section 3.3) novel policies for solving the assignment problem based on RL have been implemented (see Section 3.4). Lastly, all RL policies have been also evaluated and a comparison between them and the corresponding optimization methods has been made.

5.2 Resulting Conclusions

1. there is optimization potential even for existing methods, however business application might prove limited since it requires more computational resources and one is maybe better off with simplified version
2. RL methods prove to be very good and interesting, however being novel methods one should proceed with caution and further analyze these methods

Optimization methods are viable solutions for optimally assigning jobs to users inside workflow processes, as already argued by Zeng and Zhao [Zeng and Zhao, 2005]. Further developed policies relying on mathematical optimization done for this thesis proved indeed to yield better results (see Subsection 4.2.1), however the higher required complexity (refer to Subsection 4.4.1) poses a critical trade-off. Research Question 1 can be affirmatively answer: there is definitely

potential for further development and optimization of existing methods but further questions arise:

- Q. 1 Does a slight increase in performance justify the higher computational requirements?
- Q. 2 Can only one KPI be chosen as central parameter to evaluate a policy's performance or is a combination of different KPIs more suitable?
- Q. 3 Is it always the best solution to use only one type of optimizer or is it better to follow a more flexible approach and choose different policies on a per case basis?

All these questions must be accounted for when considering policy based optimization in workflow processes integration in IT governance.

On the other hand, RL methods demonstrate to overcome some of the problematics laid by optimization very well: 1. Generally less computationally expensive 2. Can be adopted relatively fast 3. Are generally more "dynamic" and can adapt and exploit case specific characteristics.

Then again RL methods are not exempt from disadvantages: 1. They require long training sessions in order to equal (or even outperform) optimization methods 2. When using ANNs, overfitting might lead to suboptimal solution in which policies get stuck (for viable solutions refer to [Srivastava et al., 2014]) 3. Multilayer ANNs (*i.e.*, deep ANNs) are very sensitive to VGP and EGP.

In general RL based approaches are a refreshing and novel methodology for solving optimization problems but require further development and sound domain knowledge.

5.3 Outlook

This thesis merely "scratches the surface" of viable alternatives to existing optimization techniques for workflow processes. A direct follow up consists in testing in operative workflows the efficiency measured in the simulation environment outlined in this thesis. This includes testing the robustness, efficacy and viability of the proposed policies by putting them under "real-world" stress situation in order to assert the efficiency claims. For RL methods executing lengthy training sessions might prove impractical: thousands of training sessions required by RL methods in order to comply with convergence properties can prove infeasible for companies that are not able to generate such amounts of data, thus directly limiting applicability of these methods.

RL is a novel field that is currently still being actively researched and pursued, as it has yielded promising results [Mnih et al., 2015, Silver et al., 2016]. By using ANNs one can effectively approximate nonlinear functions as it has been outlined in Subsection 3.3.6. Even though in this thesis only feedforward ANNs have been used, the problem domain is very well suited for the recurrent variant as well.

Moreover, bleeding edge domains have originated from RL such as IRL [Ng and Russell, 2000] and AL which is based on the former [Abbeel and Ng, 2004]. AL could prove to be yet another captivating approach to solve the assignment problem in which the reward function is not explicitly modeled, instead an "expert" of the domain (*i.e.*, a mathematical solver such as MSA) demonstrates a task and by means of AL the policy is trained [Abbeel and Ng, 2004].

Having said that, Research Question 2 can be answered positively as well: there are indeed state of the art approaches that can be used as alternatives or complements to the job assignment mathematical optimization.

Literature Overview

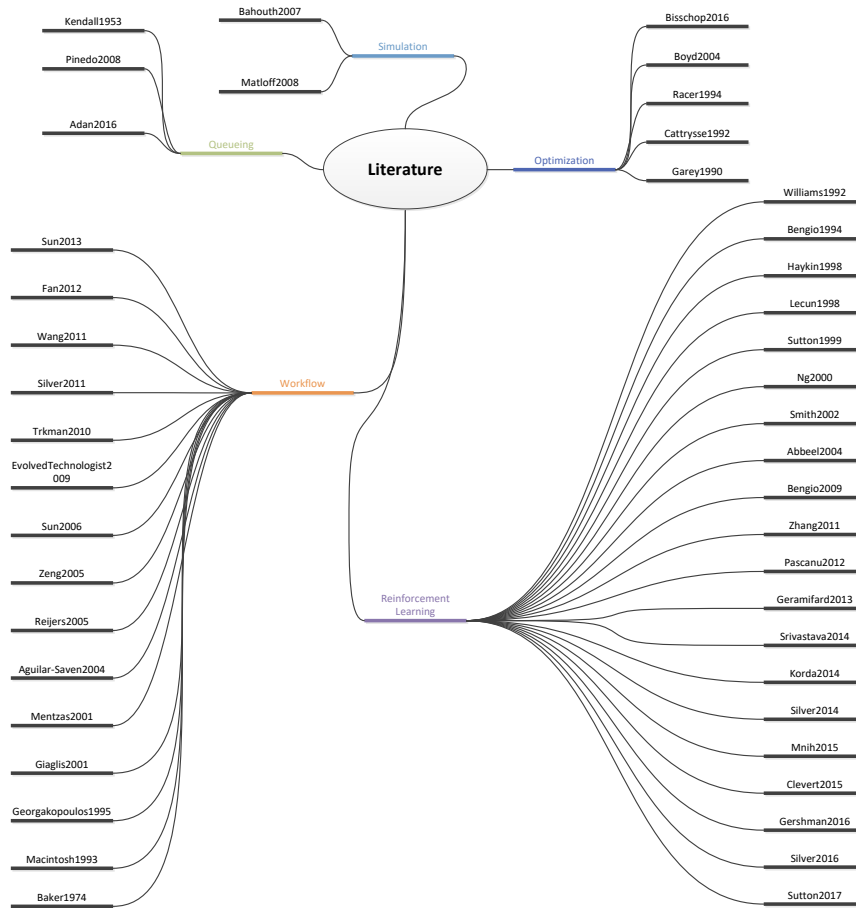


Figure A.1: Literature per topic categorization overview

Optimization Results

B.1 Least Loaded Qualified Person

B.1.1 KPIs

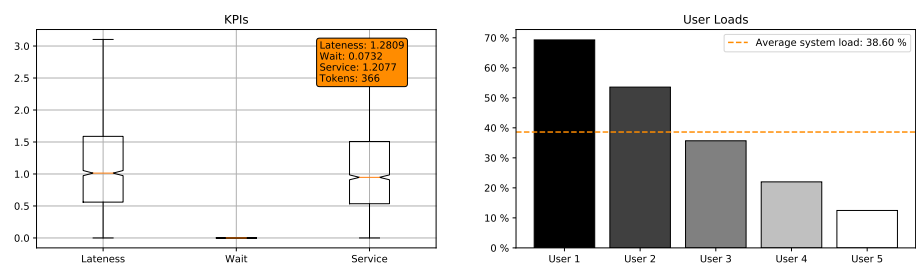


Figure B.1: LLQP KPIs

B.1.2 Evolution

B.2 Shared Queue

B.2.1 KPIs

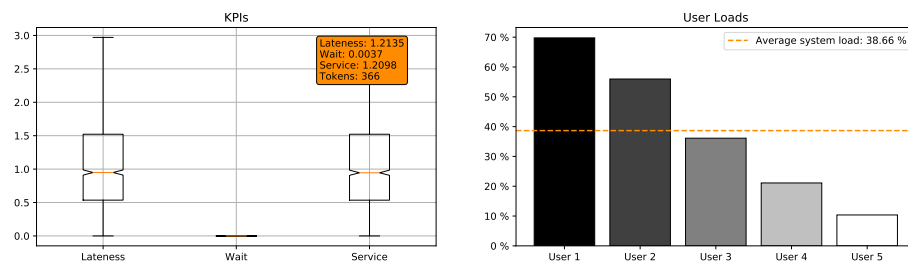


Figure B.2: SQ KPIs

B.2.2 Evolution

B.3 K-Batch

B.3.1 KPIs

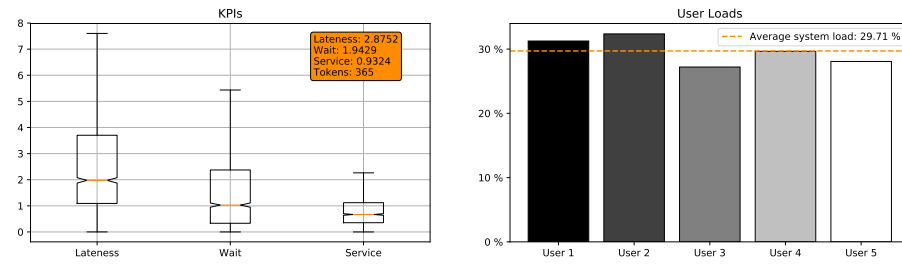


Figure B.3: K-Batch with MSA KPIs

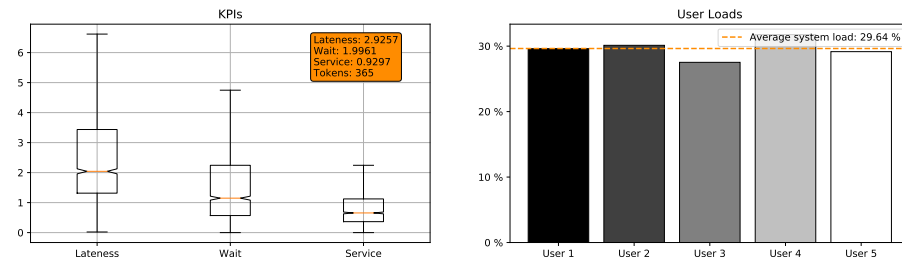


Figure B.4: K-Batch with DMF KPIs

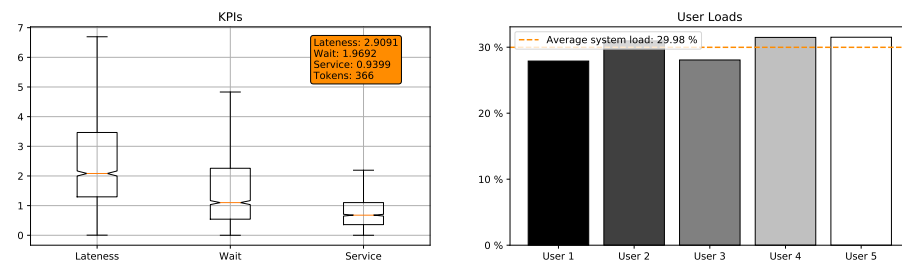
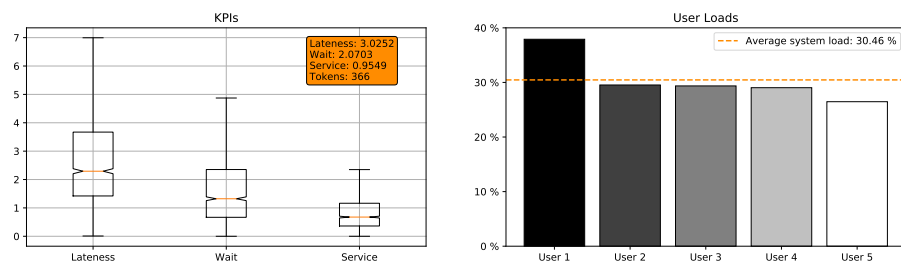
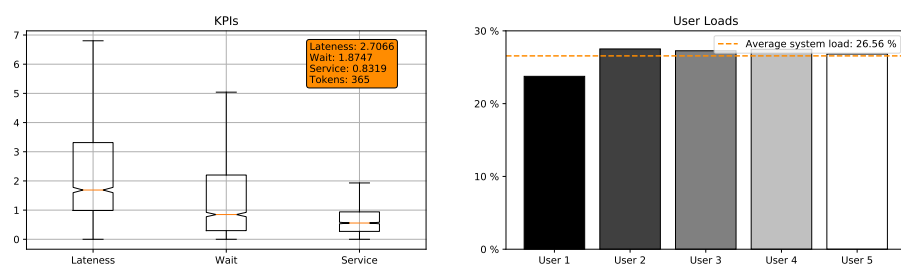


Figure B.5: K-Batch with SDMF KPIs

**Figure B.6:** K-Batch with ESDMF KPIs**Figure B.7:** K-Batch with ST KPIs

B.3.2 Evolution

B.3.3 Batch Sizes Comparison

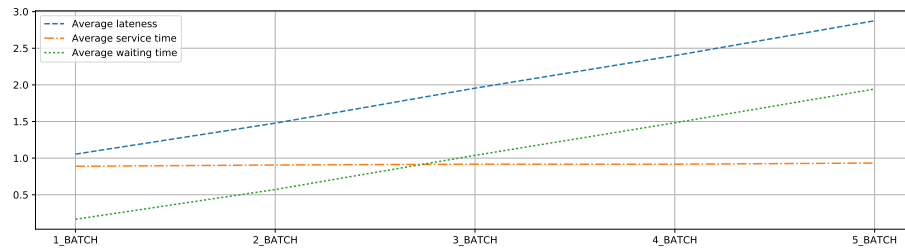


Figure B.8: K-Batch with MSA batch size comparison

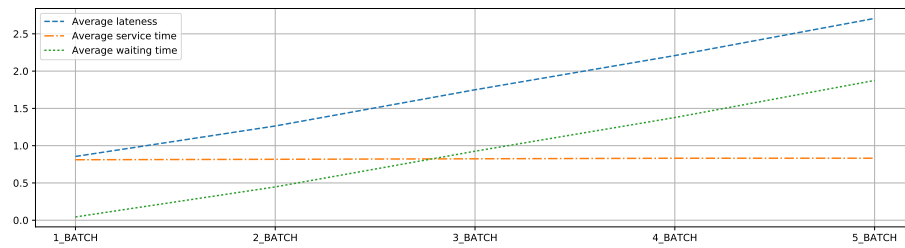


Figure B.9: K-Batch with ST batch size comparison

B.4 K-Batch-1

B.4.1 KPIs

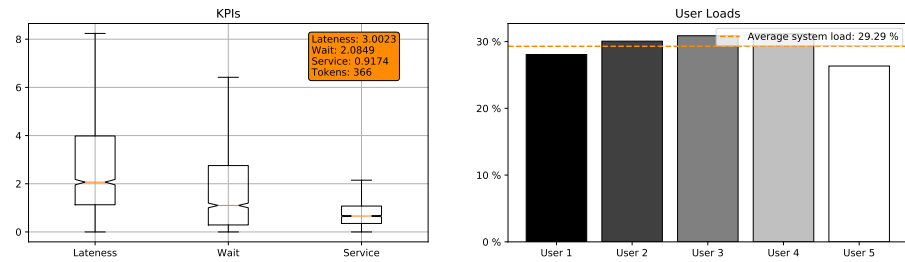


Figure B.10: K-Batch-1 with MSA KPIs

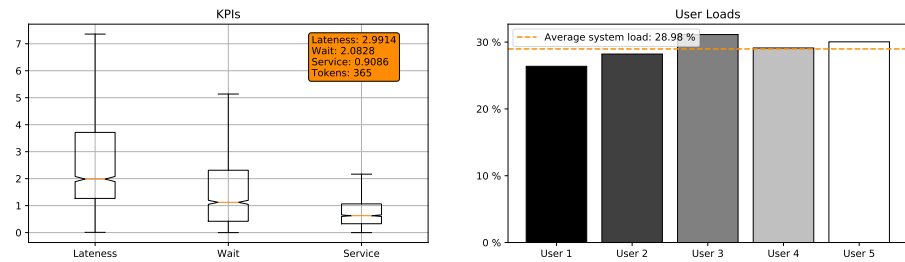


Figure B.11: K-Batch-1 with DMF KPIs

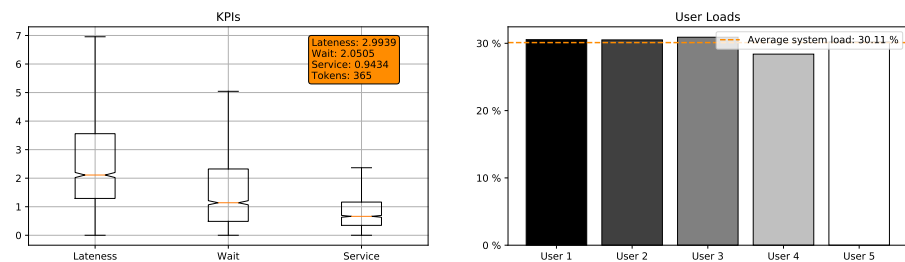


Figure B.12: K-Batch-1 with SDMF KPIs

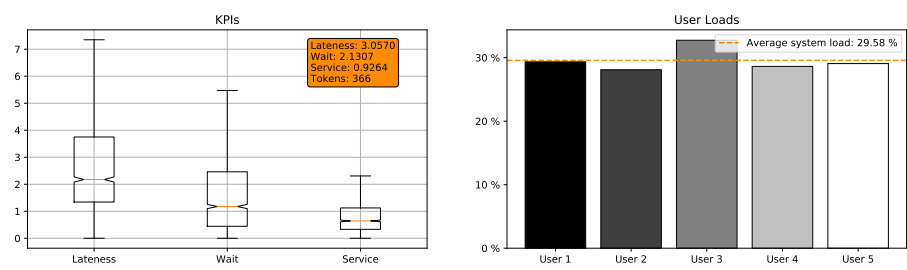


Figure B.13: K-Batch-1 with ESDMF KPIs

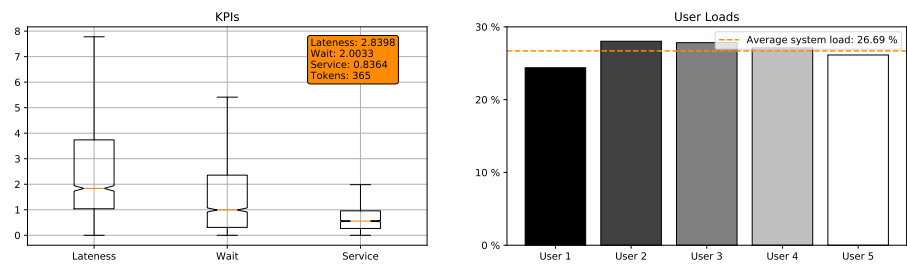


Figure B.14: K-Batch-1 with ST KPIs

B.4.2 Evolution

B.4.3 Batch Sizes Comparison

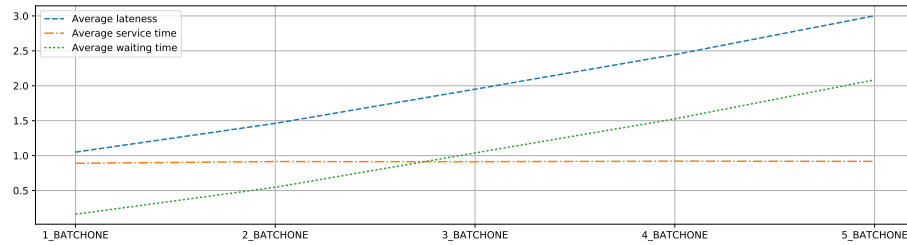


Figure B.15: K-Batch-1 with MSA batch size comparison

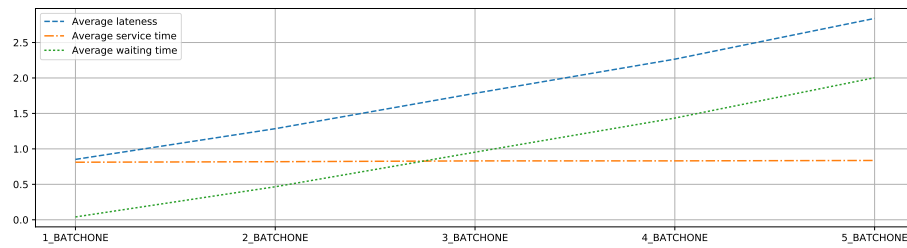


Figure B.16: K-Batch-1 with ST batch size comparison

B.5 1-Batch-1

B.5.1 KPIs

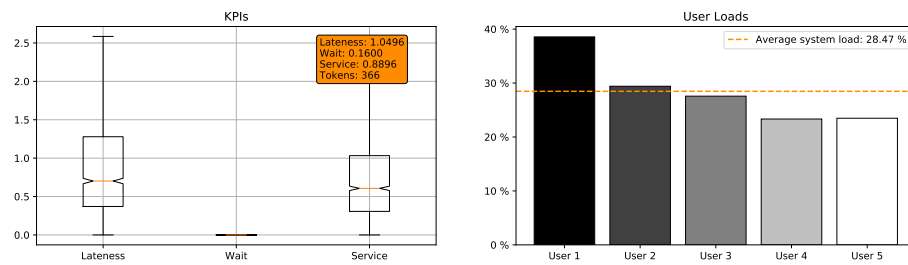


Figure B.17: 1-Batch-1 with MSA KPIs

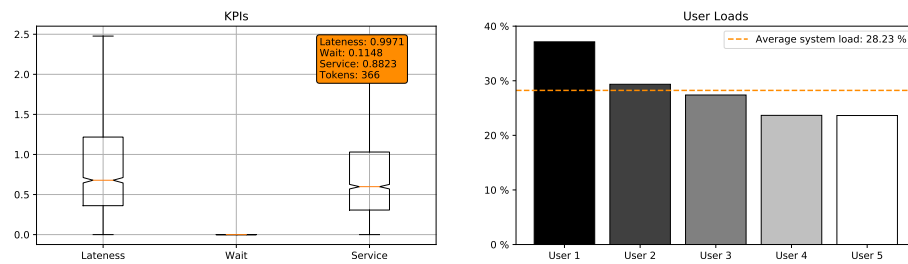


Figure B.18: 1-Batch-1 with DMF KPIs

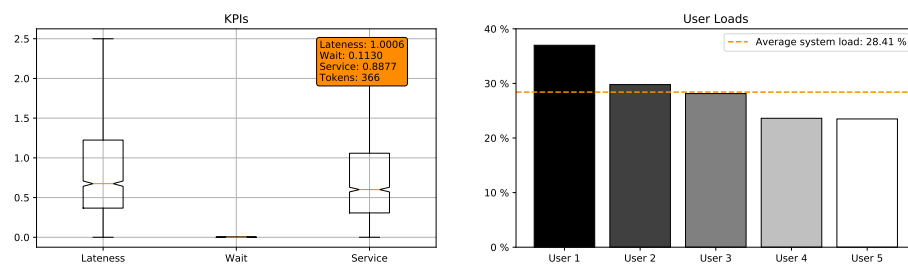


Figure B.19: 1-Batch-1 with SDMF KPIs

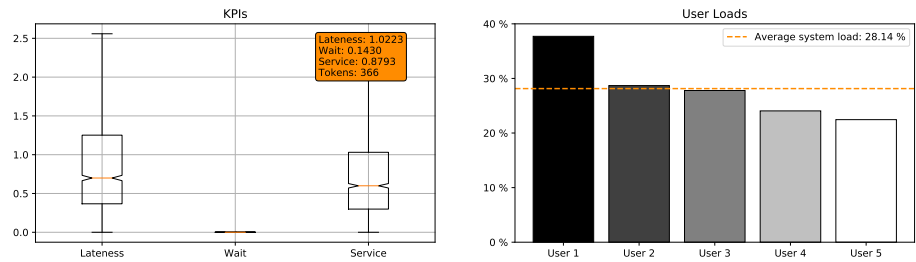


Figure B.20: 1-Batch-1 with ESDMF KPIs

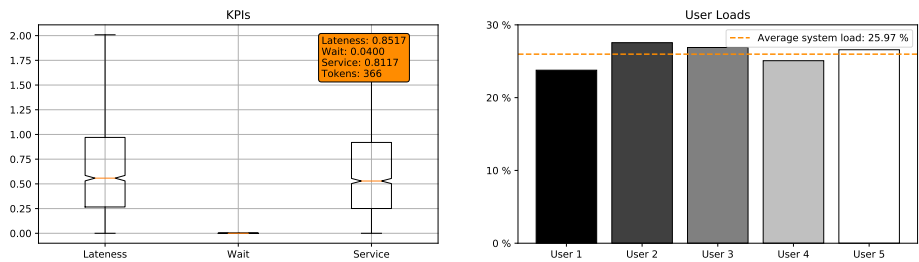


Figure B.21: 1-Batch-1 with ST KPIs

B.5.2 Evolution

Reinforcement Learning Results

C.1 1-Batch

C.1.1 KPIs

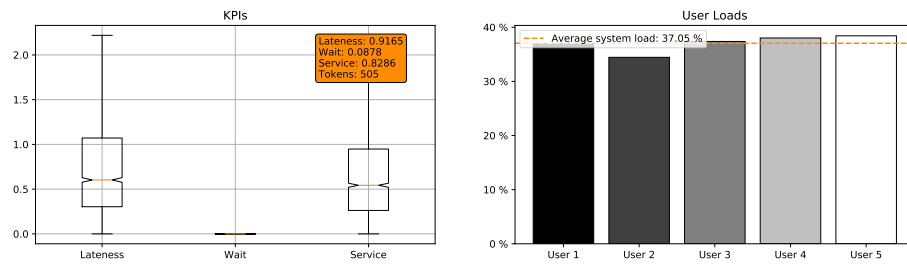


Figure C.1: 1-Batch with MC and VFA KPIs

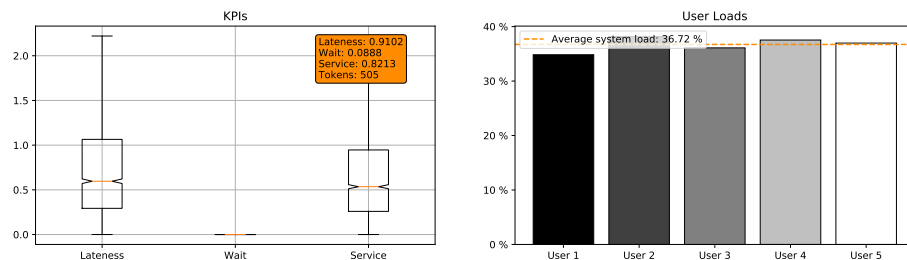


Figure C.2: 1-Batch with MC, VFA and OP KPIs

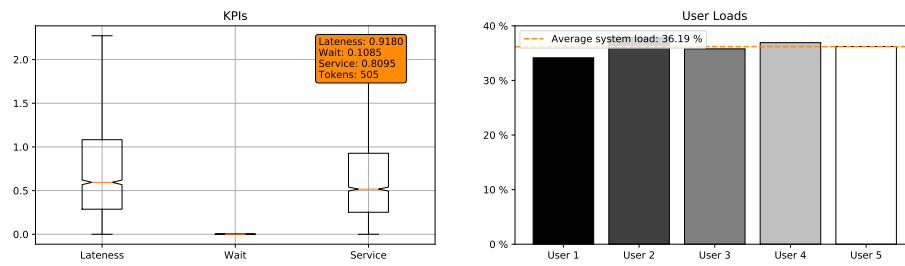


Figure C.3: 1-Batch with MC, VFA, OP and EP KPIs

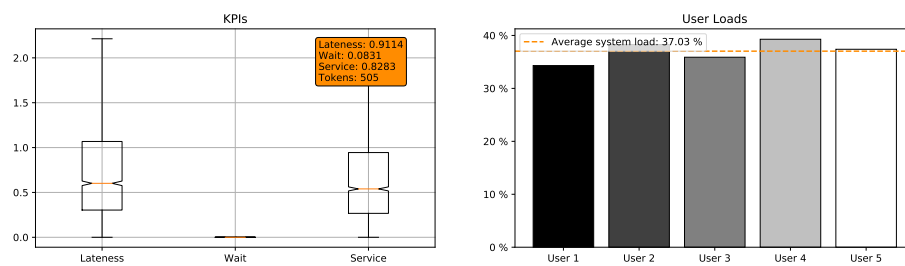


Figure C.4: 1-Batch with TD, VFA and OP KPIs

C.1.2 Evolution

C.1.3 Comparison with MSA

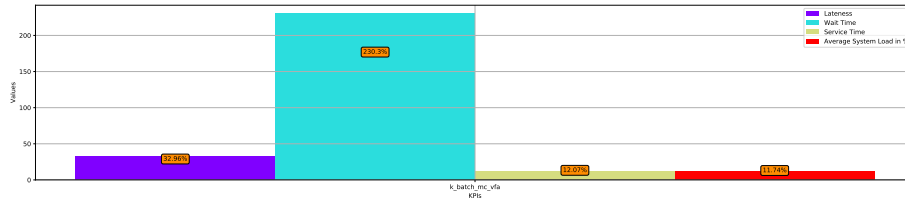


Figure C.5: 1-Batch with MC and VFA MSA comparison

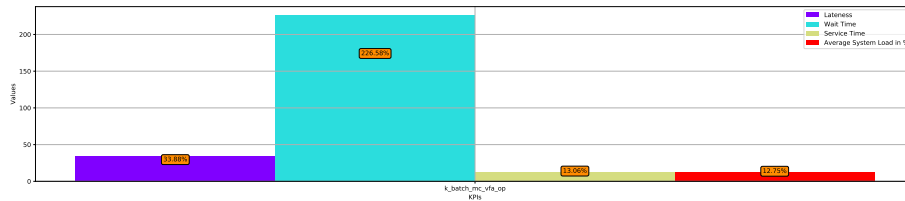


Figure C.6: 1-Batch with MC, VFA and OP MSA comparison

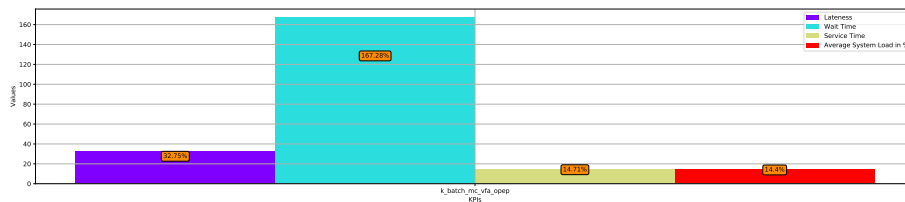


Figure C.7: 1-Batch with MC, VFA, OP and EP MSA comparison

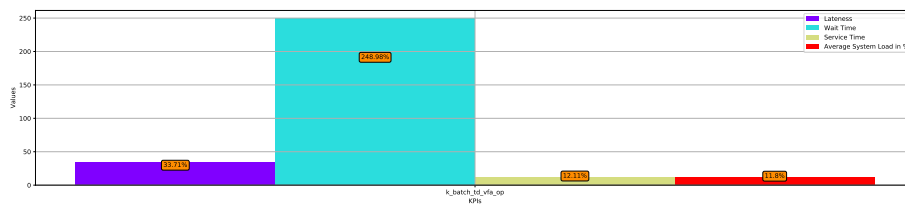


Figure C.8: 1-Batch with TD, VFA, OP and EP MSA comparison

C.2 1-Batch-1

C.2.1 KPIs

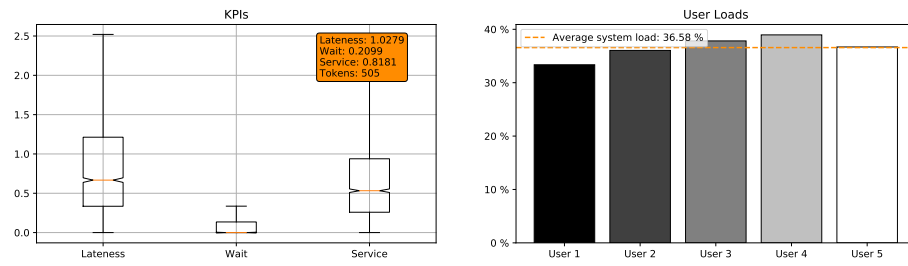


Figure C.9: 1-Batch-1 with TD, VFA and OP KPIs

C.2.2 Evolution

C.2.3 Comparison with MSA

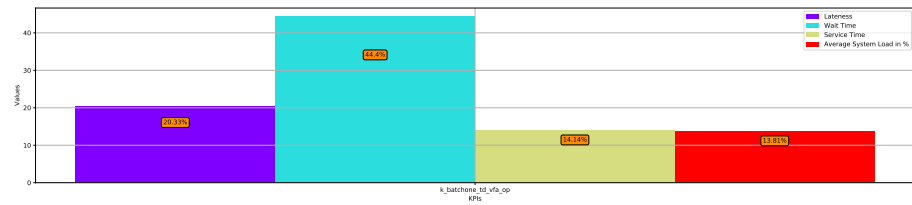


Figure C.10: 1-Batch-1 with TD, VFA and OP MSA comparison

C.3 Least Loaded Qualified Person

C.3.1 KPIs

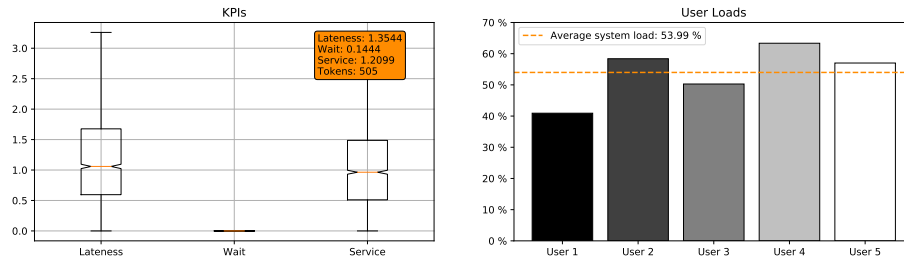


Figure C.11: LLQP with MC, VFA and OP KPIs

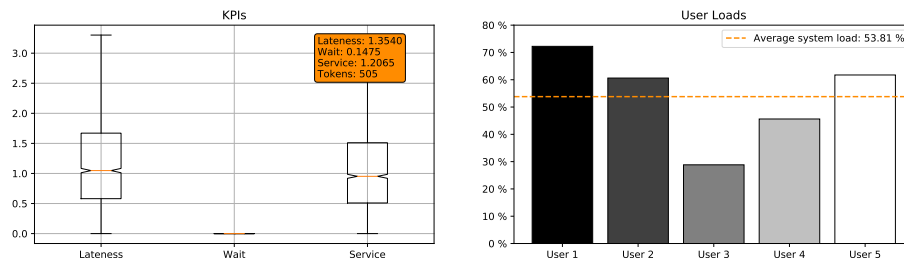


Figure C.12: LLQP with TD, VFA and OP KPIs

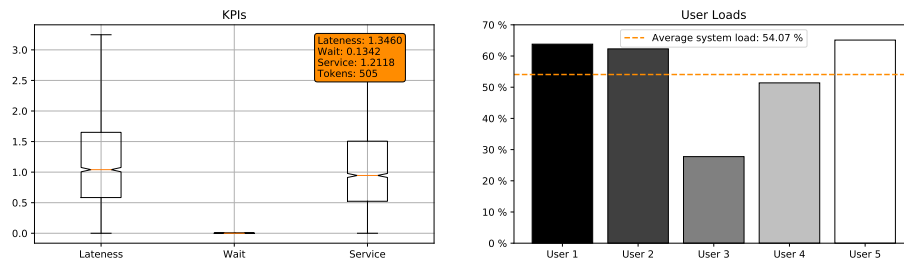


Figure C.13: LLQP with TD, TF and OP KPIs

C.3.2 Evolution

C.3.3 Comparison with MSA

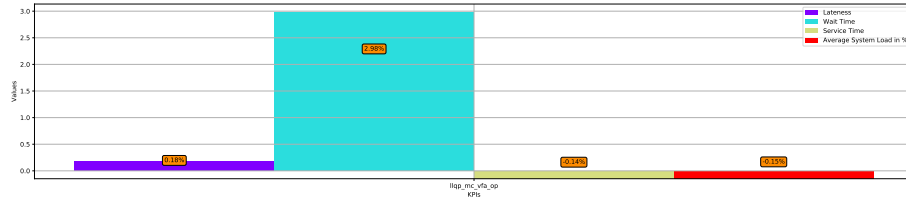


Figure C.14: LLQP with MC, VFA and OP MSA comparison

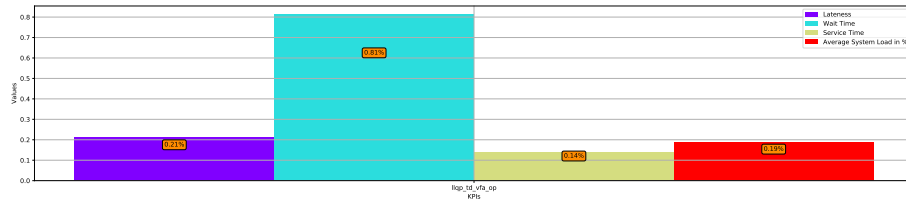


Figure C.15: LLQP with TD, VFA and OP MSA comparison

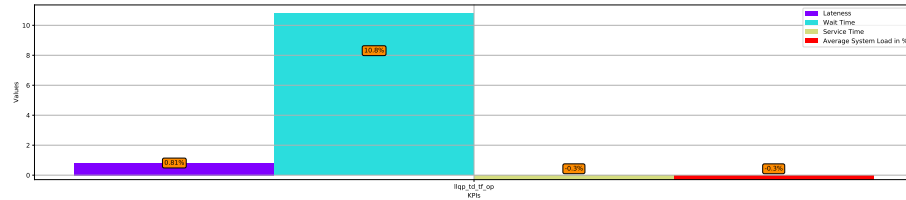


Figure C.16: LLQP with TD, TF and OP MSA comparison

C.3.4 Additional Least Loaded Qualified Person Policies

Technical Name	Policy Type	Update Method	Q Value Method	Other Characteristics
llqp_mc_vfa	LLQP	MC	VFA	None
llqp_td_vfa	LLQP	TD	VFA	None
llqp_mc_pg	LLQP	MC	PG	None
llqp_mc_pg_wb	LLQP	MC	PG	With Baseline
llqp_td_pg_ac	LLQP	TD	PG	AC
llqp_td_pg_avac	LLQP	TD	PG	AV, AC

Table C.1: Overview of additional LLQP policies with RL

C.4 Others

C.4.1 KPIs

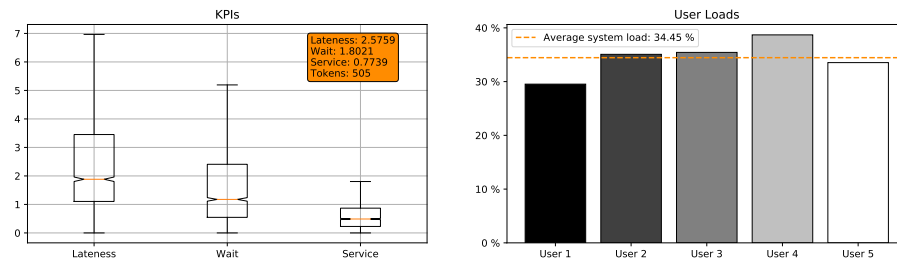


Figure C.17: WZ with TD, VFA and OP KPIs

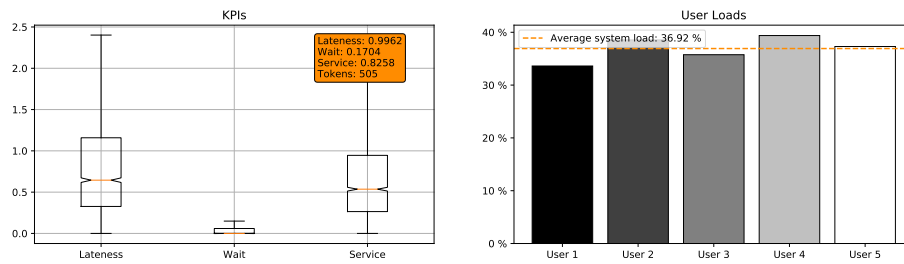


Figure C.18: WZO with TD, VFA and OP KPIs

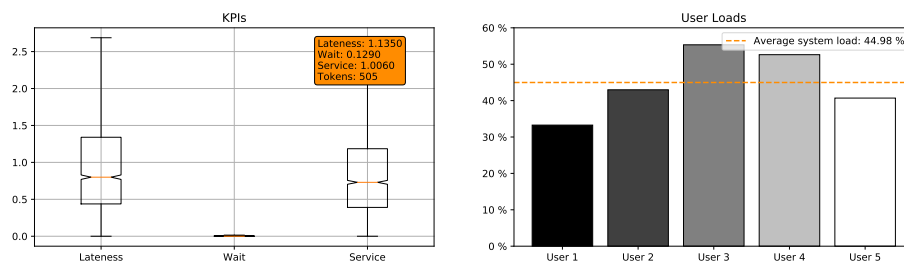


Figure C.19: BI with MC, TF and 1L KPIs

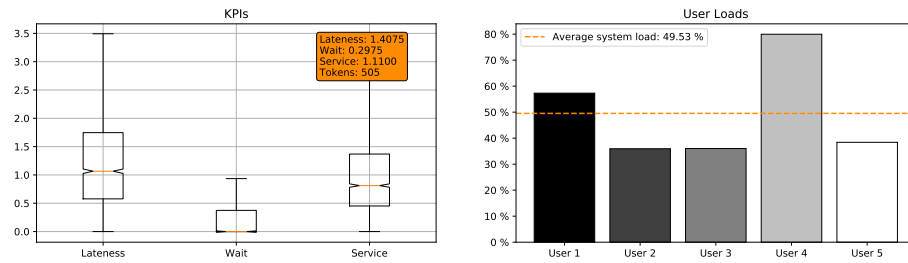


Figure C.20: BI with MC, TF and 2L KPIs

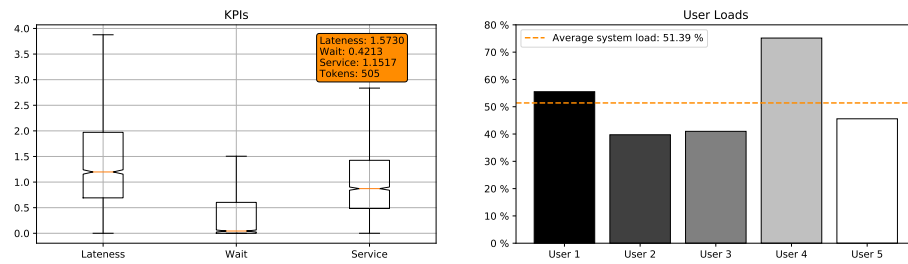


Figure C.21: BI with MC, TF and 3L KPIs

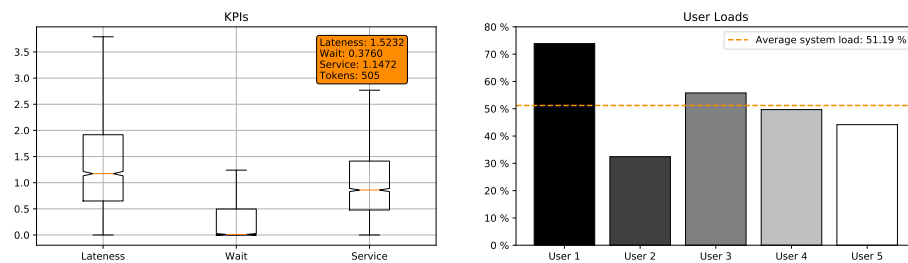


Figure C.22: BI with MC, TF and 4L KPIs

C.4.2 Evolution

C.4.3 Comparison with MSA

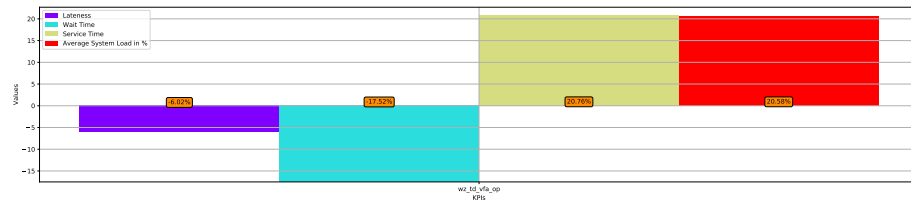


Figure C.23: WZ with TD, VFA and OP MSAs comparison

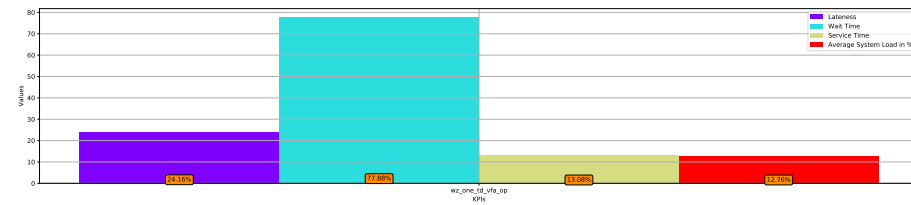


Figure C.24: WZO with TD, VFA and OP MSAs comparison

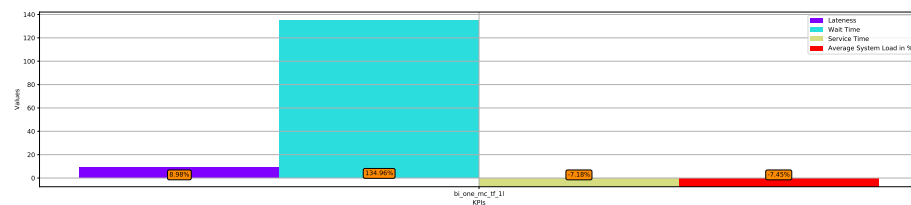


Figure C.25: BI with MC, TF and 1L MSAs comparison

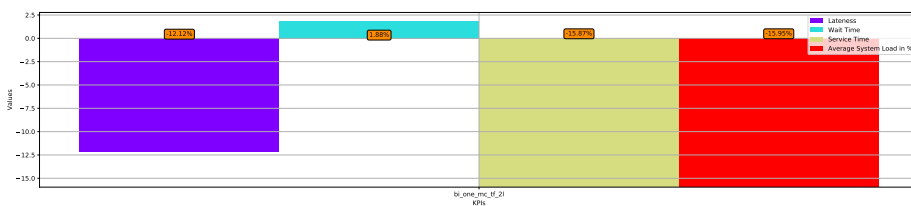


Figure C.26: BI with MC, TF and 2L MSAs comparison

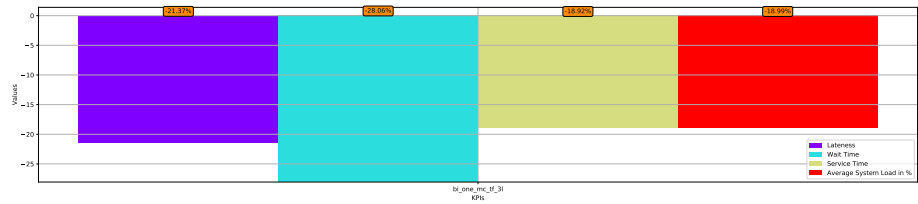


Figure C.27: BI with MC, TF and 3L MSAs comparison

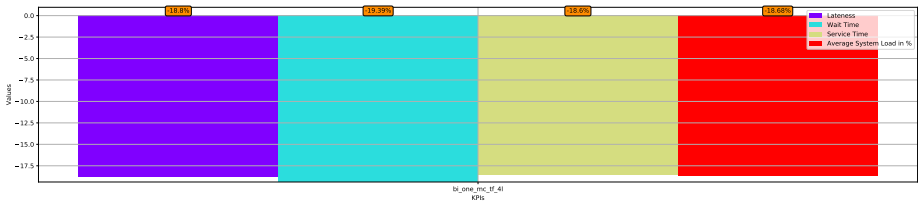


Figure C.28: BI with MC, TF and 4L MSAs comparison

Acronyms

1L One Hidden Layer for ANN. xi, 43, 76, 79

2L Two Hidden Layers for ANN. xi, 77, 79

3L Three Hidden Layers for ANN. xi, 77, 80

4L Four Hidden Layers for ANN. xi, 77, 80

AC Actor Critic. 6, 25, 26, 75

AL Apprenticeship Learning. 5, 46

ANN Artificial Neural Network. x, xi, 5, 6, 22–24, 29, 41–43, 46, 83

AV Action Value. 6, 20, 24, 25, 75

BI Batch Input One for K-Batch-1 Emulation with TF. xi, 42, 76, 77, 79, 80

BPM Business Process Management. 5

BPMN Business Process Model and Notation. 5

CSF Critical Success Factor. 5

DMF Dynamic Minimization of Maximum Task Flowtime. x, xi, 4, 7, 14–19, 34, 42, 53, 57, 61, 83, 84

EDMF Extended DMF. x, 15–17

EGP Exploding Gradient Problem. 6, 43, 46

ELU Exponential Linear Unit. 6

EP ϵ -Greedy. xi, 24, 27, 40, 66, 68

ESDMF Extremely Simplified DMF. x, xi, 18, 19, 54, 58, 62, 84

IRL Inverse RL. 5, 46

KPI Key Performance Indicator. x–xii, 3, 33, 35–44, 46, 49, 51, 53, 54, 57, 58, 61, 62, 65, 66, 69, 72, 76, 77

- LLQP** Least Loaded Qualified Person. x–xii, 4, 14, 26, 31, 40, 41, 43, 49, 72, 74, 75
- MC** Monte Carlo. x–xii, 5, 6, 20, 21, 25, 26, 29, 30, 40–42, 65, 66, 68, 72, 74–77, 79, 80
- MDP** Markov Decision Process. 6, 20
- MSA** Minimizing Sequential Assignment. x–xii, 14, 18, 19, 36–43, 46, 53, 56, 57, 60, 61, 68, 71, 74, 79, 80
- ONP** On Policy. x, xii, 21, 24, 41, 43, 44
- OP** Off Policy. x–xii, 21, 24, 40–44, 65, 66, 68, 69, 71, 72, 74, 76, 79
- PG** Policy Gradient. 5, 6, 25, 26, 28, 29, 42, 75
- ReLU** Rectified Linear Unit. 6, 22
- RL** Reinforcement Learning. xii, 1, 5, 6, 19, 21, 23, 26, 27, 31, 40–43, 45, 46, 75, 83
- SARSA** State-Action-Reward-State-Action. 21, 24
- SDMF** Simplified DMF. x, xi, 16, 17, 19, 53, 57, 61
- SGD** Stochastic Gradient Descent. 21–23, 27, 29
- SQ** Shared Queue. x, 4, 14, 51
- ST** Service Time Minimization with ESDMF as Upper Bound. x–xii, 18, 19, 37–39, 42, 43, 54, 56, 58, 60, 62
- TD** Temporal Difference. x–xii, 6, 21, 26, 29, 30, 40–43, 66, 68, 69, 71, 72, 74–76, 79
- TF** Tensorflow. xi, 29, 43, 72, 74, 76, 77, 79, 80, 83
- VFA** Value Function Approximation. xi, 5, 6, 22, 24, 27, 40–42, 65, 66, 68, 69, 71, 72, 74–76, 79
- VGP** Vanishing Gradient Problem. 5, 6, 43, 46
- WZ** Waiting Zone for K-Batch Emulation. xi, 42, 76, 79
- WZO** Waiting Zone One for K-Batch-1 Emulation. xi, 42, 43, 76, 79

Bibliography

- [Abbeel and Ng, 2004] Abbeel, P. and Ng, A. Y. (2004). Apprenticeship learning via inverse reinforcement learning. In *Proceedings of the Twenty-first International Conference on Machine Learning, ICML '04*, pages 1–, New York, NY, USA. ACM.
- [Adan and Resing, 2016] Adan, I. and Resing, J. (2016). Queueing Systems.
- [Aguilar-Savén, 2004] Aguilar-Savén, R. S. (2004). Business process modelling: Review and framework. *International Journal of Production Economics*, 90(2):129 – 149. Production Planning and Control.
- [Bahouth et al., 2007] Bahouth, A., Crites, S., Matloff, N., and Williamson, T. (2007). Revisiting the issue of performance enhancement of discrete event simulation software. In *Simulation Symposium, 2007. ANSS '07. 40th Annual*, pages 114–122.
- [Baker, 1974] Baker, K. R. (1974). *Introduction to Sequencing and Scheduling*. John Wiley & Sons.
- [Bengio, 2009] Bengio, Y. (2009). Learning deep architectures for ai. *Foundations and Trends® in Machine Learning*, 2(1):1–127.
- [Bengio et al., 1994] Bengio, Y., Simard, P., and Frasconi, P. (1994). Learning long-term dependencies with gradient descent is difficult. *Trans. Neur. Netw.*, 5(2):157–166.
- [Bisschop, 2016] Bisschop, J. (2016). AIMMS Optimization Modeling.
- [Boyd and Vandenberghe, 2004] Boyd, S. and Vandenberghe, L. (2004). *Convex Optimization*. Cambridge University Press.
- [Cattrysse and Wassenhove, 1992] Cattrysse, D. G. and Wassenhove, L. N. V. (1992). A survey of algorithms for the generalized assignment problem. *European Journal of Operational Research*, 60(3):260 – 272.
- [Clevert et al., 2015] Clevert, D.-A., Unterthiner, T., and Hochreiter, S. (2015). Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs). *ArXiv e-prints*.
- [Evolved Technologist, 2009] Evolved Technologist (2009). BPM Technology Taxonomy: A Guided Tour to the Application of BPM.
- [Fan et al., 2012] Fan, S., Zhao, J. L., Dou, W., and Liu, M. (2012). A framework for transformation from conceptual to logical workflow models. *Decision Support Systems*, 54(1):781 – 794.
- [Garey and Johnson, 1990] Garey, M. R. and Johnson, D. S. (1990). *Computers and Intractability; A Guide to the Theory of NP-Completeness*. W. H. Freeman & Co., New York, NY, USA.

- [Georgakopoulos et al., 1995] Georgakopoulos, D., Hornick, M., and Sheth, A. (1995). An overview of workflow management: From process modeling to workflow automation infrastructure. *Distributed and Parallel Databases*, 3(2):119–153.
- [Geramifard et al., 2013] Geramifard, A., Walsh, T. J., Tellex, S., Chowdhary, G., Roy, N., and How, J. P. (2013). A tutorial on linear function approximators for dynamic programming and reinforcement learning. *Found. Trends Mach. Learn.*, 6(4):375–451.
- [Gershman, 2016] Gershman, S. J. (2016). Empirical priors for reinforcement learning models. *Journal of Mathematical Psychology*, 71:1 – 6.
- [Giaglis, 2001] Giaglis, G. M. (2001). A taxonomy of business process modeling and information systems modeling techniques. *International Journal of Flexible Manufacturing Systems*, 13(2):209–228.
- [Haykin, 1998] Haykin, S. (1998). *Neural Networks: A Comprehensive Foundation*. Prentice Hall PTR, Upper Saddle River, NJ, USA, 2nd edition.
- [Kendall, 1953] Kendall, D. G. (1953). Stochastic processes occurring in the theory of queues and their analysis by the method of the imbedded markov chain. *The Annals of Mathematical Statistics*, 24(3):338–354.
- [Korda and Prashanth, 2014] Korda, N. and Prashanth, L. A. (2014). On TD(0) with function approximation: Concentration bounds and a centered variant with exponential convergence. *ArXiv e-prints*.
- [Lecun et al., 1998] Lecun, Y., Bottou, L., Bengio, Y., and Haffner, P. (1998). Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324.
- [Macintosh, 1993] Macintosh, A. L. (1993). The need for enriched knowledge representation for enterprise modelling. In *IEE Colloquium on AI (Artificial Intelligence) in Enterprise Modelling*, pages 3/1–3/3.
- [Matloff, 2008] Matloff, N. (2008). Introduction to discrete-event simulation and the simpy language.
- [Mentzas et al., 2001] Mentzas, G., Halaris, C., and Kavadias, S. (2001). Modelling business processes with workflow systems: an evaluation of alternative approaches. *International Journal of Information Management*, 21(2):123 – 135.
- [Mnih et al., 2015] Mnih, V., Kavukcuoglu, K., Silver, D., Rusu, A. A., Veness, J., Bellemare, M. G., Graves, A., Riedmiller, M., Fidjeland, A. K., Ostrovski, G., Petersen, S., Beattie, C., Sadik, A., Antonoglou, I., King, H., Kumaran, D., Wierstra, D., Legg, S., and Hassabis, D. (2015). Human-level control through deep reinforcement learning. *Nature*, 518(7540):529–533. Letter.
- [Ng and Russell, 2000] Ng, A. Y. and Russell, S. J. (2000). Algorithms for inverse reinforcement learning. In *Proceedings of the Seventeenth International Conference on Machine Learning, ICML '00*, pages 663–670, San Francisco, CA, USA. Morgan Kaufmann Publishers Inc.
- [Pascanu et al., 2012] Pascanu, R., Mikolov, T., and Bengio, Y. (2012). Understanding the exploding gradient problem. *CoRR*, abs/1211.5063.
- [Pinedo, 2008] Pinedo, M. L. (2008). *Scheduling: Theory, Algorithms, and Systems*. Springer Publishing Company, Incorporated, 3rd edition.

- [Racer and Amini, 1994] Racer, M. and Amini, M. M. (1994). A robust heuristic for the generalized assignment problem. *Annals of Operations Research*, 50(1):487–503.
- [Reijers and van der Aalst, 2005] Reijers, H. A. and van der Aalst, W. M. (2005). The effectiveness of workflow management systems: Predictions and lessons learned. *International Journal of Information Management*, 25(5):458 – 472.
- [Silver, 2011] Silver, B. (2011). *BPMN Method and Style: With BPMN Implementer’s Guide*. Cody-Cassidy Press.
- [Silver et al., 2016] Silver, D., Huang, A., Maddison, C. J., Guez, A., Sifre, L., van den Driessche, G., Schrittwieser, J., Antonoglou, I., Panneershelvam, V., Lanctot, M., Dieleman, S., Grewe, D., Nham, J., Kalchbrenner, N., Sutskever, I., Lillicrap, T., Leach, M., Kavukcuoglu, K., Graepel, T., and Hassabis, D. (2016). Mastering the game of go with deep neural networks and tree search. *Nature*, 529(7587):484–489. Article.
- [Silver et al., 2014] Silver, D., Lever, G., Heess, N., Degris, T., Wierstra, D., and Riedmiller, M. (2014). Deterministic policy gradient algorithms. *Journal of Machine Learning Research*.
- [Smith, 2002] Smith, A. J. (2002). Applications of the self-organising map to reinforcement learning. *Neural Networks*, 15(8–9):1107 – 1124.
- [Srivastava et al., 2014] Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. (2014). Dropout: A simple way to prevent neural networks from overfitting. *Journal of Machine Learning Research*, 15:1929–1958.
- [Sun and Zhao, 2013] Sun, S. X. and Zhao, J. L. (2013). Formal workflow design analytics using data flow modeling. *Decision Support Systems*, 55(1):270 – 283.
- [Sun et al., 2006] Sun, S. X., Zhao, J. L., Nunamaker, J. F., and Sheng, O. R. L. (2006). Formulating the data-flow perspective for business process management. *Info. Sys. Research*, 17(4):374–391.
- [Sutton and Barto, 2017] Sutton, R. S. and Barto, A. G. (2017). *Reinforcement Learning: An Introduction*. The MIT Press.
- [Sutton et al., 1999] Sutton, R. S., McAllester, D. A., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation.
- [Trkman, 2010] Trkman, P. (2010). The critical success factors of business process management. *International Journal of Information Management*, 30(2):125 – 134.
- [Wang and Zhao, 2011] Wang, H. J. and Zhao, J. L. (2011). Constraint-centric workflow change analytics. *Decision Support Systems*, 51(3):562 – 575.
- [Williams, 1992] Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Mach. Learn.*, 8(3-4):229–256.
- [Zeng and Zhao, 2005] Zeng, D. D. and Zhao, J. L. (2005). Effective role resolution in workflow management. 17(3):374–387.
- [Zhang and Hyvärinen, 2011] Zhang, K. and Hyvärinen, A. (2011). A general linear non-gaussian state-space model: Identifiability, identification, and applications. In *Asian Conference on Machine Learning*, volume 20, pages 113–128. JMLR: Workshop and Conference Proceedings.