Learning Linear Composite Dispatch Rules for Scheduling

Case study for the job-shop problem

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Abstract Needs a rewrite

Instead of creating new dispatching rules in an ad-hoc manner, this study gives a framework on how to analyse heuristics for scheduling problems. Before starting to create new composite priority dispatching rules, meticulous research on optimal schedules can give an abundance of valuable information that can be utilised for learning new models. For instance, it's possible to seek out when the scheduling process is most susceptible to failure. Furthermore, the stepwise optimality of individual features imply their explanatory predictability. From which, a preference set is collected and a preference based learning model is created based on what feature states are preferable to others w.r.t. the end result, here minimising the final makespan. By doing so it's possible to learn new composite priority dispatching rules that outperform the models they are based on. Even though this study is based around the jobshop scheduling problem, it can be generalised to any kind of combinatorial problem.

 $\textbf{Keywords} \ \ \text{Scheduling} \cdot \text{Composite dispatching rules} \cdot \text{Machine Learning} \cdot \text{Feature Selection}$

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1 Introduction

The introduction must be completely re-written to reflect what was done in this paper.) – Ongoing

The problem is to learn new problem specific priority dispatching rules for scheduling. A subclass of scheduling problems is the job-shop scheduling problem (JSP), which is widely studied in operations research. JSP deals with the allocation of tasks of competing resources where its goal is to optimise a single or multiple objectives. Its analogy is from manufacturing industry where a set of jobs are broken down into tasks that must be processed on several machines in a workshop. Furthermore, its formulation can be applied on a wide variety of practical problems in real-life applications which involve decision making, therefore its problem-solving capabilities has a high impact on many manufacturing organisations.

In order to find an optimal (or near optimal) solution for scheduling problems one could either use exact methods or heuristics methods. Exact methods guarantee an optimal solution, however, job-shop scheduling is strongly NP-hard [5]. Any exact algorithm generally suffers from the curse of dimensionality, which impedes the application in finding the global optimum in a reasonable amount of time. Heuristics are generally more time efficient but do not necessarily attain the global optimum. Therefore, job-shop has the reputation of being notoriously difficult to solve. As a result, it's been widely studied in deterministic scheduling theory and its class of problems has been tested on a plethora of different solution methodologies from various research fields [19], all from simple and straight forward dispatching rules to highly sophisticated frameworks.

Generally, job-shop is solved by applying a hand-crafted dispatching rule (DR) for a given problem space. Due to the exorbitant amounts of DRs to choose from, and any kind of alteration to the problem space, this can become quite a time-consuming selection process for the heuristic designer, which any kind of automation would alleviate immensely. With meta heuristics one can use existing DRs, and use for example portfolio-based algorithm selection [25,6], either based on a single instance or class of instances [33] to determine which DR to choose from. Implementing ant colony optimisation to select the best DR from a selection of nine DRs for JSP, experiments from [15] showed that the choice of DR do affect the results and that for all performance measures considered. They showed that it was better to have a all the DRs to choose from rather than just a single DR at a time. Combining dispatching rules, with the aid of genetic programming (GP), results from [31] were promising compared to the benchmarks DRs from the literature. The main drawback, is that the rules from their GP framework is quite complex, and difficult to contrive a meaningful description to a layman.

Heuristics algorithms for scheduling are typically either a construction or improvement heuristics. The improvement heuristic starts with a complete schedule and then tries to find similar, but better schedules. A construction heuristic starts with an empty schedule and adds one job at a time until the schedule is complete. The work presented here will focus on construction heuristics, dispatching rules, although the techniques developed could be adapted to improvement heuristics also.

Direct search (GA based, Poli, etc)

A novel iterative dispatching rules that were evolved with GP for JSP, [21] learned from completed schedules in order to iteratively improve new ones. At each dispatching step, the method can utilise the current feature space to *correctify* some possible *bad* dispatch made previously (sort of reverse lookahead). Their method is straightforward, and thus easy to implement and more importantly computationally inexpensive, although the authors do stress that there is still remains room for improvement.

In the field of Artificial Intelligence, [19] point out that despite their 'intelligent' solutions, the effectiveness of finding the optimum has been rather limited. However, combined with local-search methodologies, they can be improved upon significantly, as [19] showed with the use of a hybrid method using Genetic Algorithms (GA) and Tabu Search (TS). Therefore, getting the best of both worlds, namely, the diverse global search obtained from GA and being complemented with the intensified local search capabilities of TS. Now, hybridisation of global and local methodologies is non-trivial. In general combination of the two improves performance, however, they often come at a great computational cost.

Cite Poli here!

Reinforcement learning based, Diettrich, also Kendall & Burke

Using improvement heuristics, [35] studied space shuttle payload processing by using reinforcement learning (RL), in particular, temporal difference learning. Starting with a relaxed problem, each job was scheduled as early as its temporal partial order would permit, there by initially ignoring any resource constraints on the machines, yielding the schedule's critical path. Then the schedule would be repaired so the resource constraints were satisfied in the minimum amount of iterations.

Meta learning can be very fruitful in RL, as experiments from [14] discovered some key discriminants between competing algorithms for their particular problem instances, which provided them with a hybrid algorithm which combines the strengths of the algorithms.

Cite Burke here!

Using case based reasoning for timetable scheduling, training data in [1] is guided by the two best heuristics in the literature. They point out that in order for their framework to be successful, problem features need to be sufficiently explanatory and training data need to be selected carefully so they can suggest the appropriate solution for a specific range of new cases. Again, stressing the importance of meaningful feature selection.

Supervised learning (Siggi, etc) – concentrate on this!

A recent editorial of the state-of-the-art approaches in advanced dispatching rules for large-scale manufacturing systems by [2] points out that: "... most traditional dispatching rules are based on historical data. With the emergence of data mining and on-line analytic processing, dispatching rules can now take predictive information into account." The importance of automated discovery of DR was also emphasised by [20]. Several of successful implementations in the field of semiconductor wafer

fabrication facilities are discussed, however, this sort of investigation is still in its infancy.

The alternative to hand-crafting heuristics, is to implement an automatic way of learning heuristics using a data driven approach. Data can be generated using a known heuristic, such an approach is taken in [16] for job-shop where a LPT-heuristic is applied. Afterwards, a decision tree is used to create a dispatching rule with similar logic. However, this method cannot outperform the original LPT-heuristic used to guide the search. For instruction scheduling, this drawback is confronted in [18,29, 22] by using an optimal scheduler, computed off-line. The optimal solutions are used as training data and a decision tree learning algorithm applied as before. Preferring simple to complex models, the resulting dispatching rules gave significantly better schedules than using popular heuristics in that field, and a lower worst-case factor from optimality.

The focus on this study is better understanding of *how* and *when* dispatching rules work in general, in order to mediate the set-up for the learning problem. For this reason, we propose a framework for learning the indicators of optimal solutions, such as done by [22], as an in-depth analysis of a expert policy gives a benchmark of what is theoretically possible to learn.

The study shows that during the scheduling process, it varies *when* it's most fruitful to make the 'right' decision, and depending on the problem space those pivotal moments can vary greatly.

Although, using optimal trajectory for creating training data gives vital information on how to learn good scheduling rules, it is a good starting point, but not sufficient. This is due to the fact our models are only based on optimal decisions, then once we make a suboptimal choice we are in uncharted territory and its effects are relatively unknown. For this reason, it is of paramount importance to inspect the actual end-performance when choosing a suitable model, not just staring blindly at the validation accuracy. Moreover, different measures on how to report training accuracy is discussed.

Outline of paper

The outline of the paper is the following, Section 2 gives the mathematical formalities of the scheduling problem, and Section 3 describes the main attributes for job-shop, and goes into how to create schedules with dispatching rules. In Section 4 we show how to create composite priority dispatching rules using preference learning, focusing on how to compare operations and collect training data. Section 5 sets up the framework for learning from optimal schedules. In particular, the probability of choosing optimal decisions and the effects of making a suboptimal decision. Furthermore, the optimality of common single priority dispatching rules is investigated. With those guidelines, Section 6 goes into detail how to create meaningful composite priority dispatching rules, with the importance of good feature selection and the polysemy of how to report accuracy. The paper finally concludes in Section 7 with discussion and conclusions.

2 Job-shop Scheduling

The job-shop problem (JSP) involves the scheduling of jobs on a set of machines. Each job consists of a number of operations which are then processed on the machines in a predetermined order. An optimal solution to the problem will depend on the specific objective.

In this study we will consider the $n \times m$ JSP, where n jobs, $\mathscr{J} = \{J_j\}_{j=1}^n$, are scheduled on a finite set, $\mathscr{M} = \{M_a\}_{a=1}^m$, of m machines. The index j refers to a job $J_j \in \mathscr{J}$ while the index a refers to a machine $M_a \in \mathscr{M}$. If a job requires a number of processing steps or operations, then the pair (j,a) refers to the operation, i.e., processing the task of job J_j on machine M_a .

Each job J_j has an indivisible operation time (or cost) on machine M_a , p_{ja} , which is assumed to be integral and finite. Starting time of job J_j on machine M_a is denoted $x_s(j,a)$ and its end time is denoted $x_e(j,a)$ where,

$$x_e(j,a) := x_s(j,a) + p_{ja}$$
 (1)

Each job J_j has a specified processing order through the machines, it is a permutation vector, σ_j , of $\{1,...,m\}$, representing a job J_j can be processed on $M_{\sigma_j(a)}$ only after it has been completely processed on $M_{\sigma_i(a-1)}$, i.e.,

$$x_s(j, \mathbf{\sigma}_i(a)) \ge x_e(j, \mathbf{\sigma}_i(a-1))$$
 (2)

for all $J_j \in \mathcal{J}$ and $a \in \{2,...,m\}$. Note, that each job can have its own distinctive flow pattern through the machines, which is independent of the other jobs. However, in the case that all jobs share the same *fixed* permutation route, it will be referred to as FSP.

The disjunctive condition that each machine can handle at most one job at a time is the following,

$$x_s(j,a) \ge x_e(j',a)$$
 or $x_s(j',a) \ge x_e(j,a)$ (3)

for all $J_j, J_{j'} \in \mathcal{J}$, $J_j \neq J_{j'}$ and $M_a \in \mathcal{M}$.

The objective function is to minimise its maximum completion times for all tasks, commonly referred to as the makespan, C_{max} , which is defined as follows,

$$C_{\max} := \max\{x_e(j, \boldsymbol{\sigma}_i(m)) \mid J_i \in \mathcal{J}\}. \tag{4}$$

Additional constraints commonly considered are job release-dates and due-dates or sequence dependent set-up times, however, these will not be considered here. This family of scheduling problems is denoted by $J||C_{\text{max}}|$ [24].

Here we must say something about the computational complexity of the $J||C_{\text{max}}$ compared to other scheduling problems, and why we consider only this one in our study. It may be useful to look at Pinedo also on this subject ... perhaps also mention that many of the dispatching rules in the literature have been designed around this problem... use this to tie to he next section – OK?

Deterministic JSP is the most *general* case for classical scheduling problems [12]. Many other scheduling problems can be reformulated as JSP. For instance the widely studied Travelling Salesman Problem can be contrived as job-shop with the salesman

as a single machine in use and the cities to be visited are the jobs to be processed. Moreover, the general form of JSP assumes that each job can have its own distinctive flow pattern through the machines, which is independent of the other jobs. In the case where all jobs share the same permutation route, job-shop is reduced to a permutation flow-shop scheduling problem [7,31]. Therefore, without loss of generality, this study is structured around JSP.

3 Priority Dispatching Rules

Priority dispatching rules determine, from a list of incomplete jobs, \mathcal{L} , which job should be dispatched next. This process is illustrated in Figure 1, where an example of a temporal partial schedule of six-jobs scheduled on five-machines is given. The numbers in the boxes represent the job identification j. The width of the box illustrates the processing times for a given job for a particular machine M_a (on the vertical axis). The dashed boxes represent the resulting partial schedule for when a particular job is scheduled next. Moreover, the current C_{max} is denoted by a dotted vertical line. The object is to keep this value as small as possible once all operations are complete. As shown in the example there are 15 operations already scheduled. The *sequence* of dispatches used to create this partial schedule is,

$$\chi = (J_3, J_3, J_3, J_4, J_4, J_5, J_1, J_1, J_2, J_4, J_6, J_4, J_5, J_3)$$
(5)

and refers to the sequential ordering of job dispatches to machines, i.e., (j,a); the collective set of allocated jobs to machines is interpreted by its sequence, is referred to as a *schedule*. A *scheduling policy* will pertain to the manner in which the sequence is determined from the available jobs to be scheduled. In our example the available jobs is given by the job-list $\mathcal{L}^{(k)} = \{J_1, J_2, J_4, J_5, J_6\}$ with the five potential jobs to be dispatched at step k = 16 (note that J_3 is completed).

Deciding which job to dispatch is, however, not sufficient, one must also know where to place it. In order to build tight schedules it is sensible to place a job as soon as it becomes available and such that the machine idle time is minimal, i.e., schedules are non-delay. There may also be a number of different options for such a placement. In Fig. 1 one observes that J_2 , to be scheduled on M_3 , could be placed immediately in a slot between J_3 and J_4 , or after J_4 on this machine. If J_6 had been placed earlier, a slot would have been created between it and J_4 , thus creating a third alternative, namely scheduling J_2 after J_6 . The time in which machine M_a is idle between consecutive jobs J_j and $J_{j'}$ is called idle time, or flow,

$$f(a,j) := x_s(j,a) - x_e(j',a)$$
 (6)

where J_i is the immediate successor of $J_{i'}$ on M_a .

Construction heuristics are designed in such a way that it limits the search space in a logical manner, respecting not to exclude the optimum. Here, the construction heuristic is to schedule the dispatches as closely together as possible, i.e., minimise the schedule's flow. More specifically, once an operation (j,a) has been chosen from the job-list, \mathcal{L} , by some dispatching rule, it can placed immediately after (but not

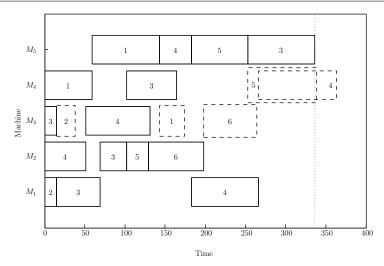


Fig. 1 Gantt chart of a partial JSP schedule after 15 dispatches: Solid and dashed boxes represent χ and $\mathcal{L}^{(16)}$, respectively. Current C_{max} denoted as dotted line.

prior) $x_e(j, \sigma_j(a-1))$ on machine M_a due to constraint Eq. (2). However to guarantee that constraint Eq. (3) is not violated, idle times M_a are inspected, as they create flow time which J_j can occupy. Bearing in mind that J_j release time is $x_e(j, \sigma_j(a-1))$ one cannot implement Eq. (6) directly, instead it has to be updated as follows,

$$\tilde{f}(a,j') := x_s(j'',a) - \max\{x_e(j',a), x_e(j, \mathbf{\sigma}_i(a-1))\}$$
(7)

for all already dispatched jobs $J_{j'}, J_{j''} \in \mathscr{J}_a$ where $J_{j''}$ is $J_{j'}$ successor on M_a . Since pre-emption is not allowed, the only applicable slots are whose idle time can process the entire operation, i.e.,

$$\tilde{F}_{ja} := \left\{ J_{j'} \in \mathscr{J}_a \mid \tilde{f}(a, j') \ge p_{ja} \right\}. \tag{8}$$

The placement rule applied will decide where to place the job and is an intrinsic heuristic of the construction heuristic, chosen independently of the priority dispatching rule applied. Different placement rules could be considered for selecting a slot from Eq. (8), e.g., if the main concern were to utilise the slot space, then choosing the slot with the smallest idle time would yield a closer-fitted schedule and leaving greater idle times undiminished for subsequent dispatches on M_a . In our experiments cases were discovered where such a placement can rule out the possibility of constructing optimal solutions. This problem, however, did not occur when jobs are simply placed as early as possible, which is beneficial for subsequent dispatches for J_j . For this reason it will be the placement rule applied here.

Priority dispatching rules will use attributes of operations, such as processing time, in order to determine the job with the highest priority. Consider again Figure 1, if the job with the shortest processing time (SPT) were to be scheduled next, then J_2 would be dispatched. Similarly, for the longest processing time (LPT) heuristic, J_5 would have the highest priority. Dispatching can also be based on attributes related

Inconsist: attribute versus feature

Table 1 Attribute space \mathscr{A} for JSP where job J_j on machine M_a given the resulting temporal schedule after operation (j,a).

φ	Feature description	Mathematical formulation	Shorthand					
job related								
ϕ_1	job processing time	p_{ja}	proc					
ϕ_2	job start-time	$x_s(j,a)$	startTime					
ϕ_3	job end-time	$x_e(j,a)$	endTime					
ϕ_4	job arrival time	$x_e(j,a-1)$	arrival					
ϕ_5	time job had to wait	$x_s(j,a) - x_e(j,a-1)$	wait					
ϕ_6	total processing time for job	$\sum_{a\in\mathscr{M}}p_{ja}$	jobTotProcTime					
ϕ_7	total work remaining for job	$\sum_{a' \in \mathcal{M} \setminus \mathcal{M}_j} p_{ja'}$	jobWrm					
ϕ_8	number of assigned operations for job	$ \mathscr{M}_j $	jobOps					
	machine related							
ϕ_9	when machine is next free	$\max_{j' \in \mathcal{J}_a} \{ x_e(j', a) \}$	macFree					
ϕ_{10}	total processing time for machine	$\sum_{j\in\mathscr{J}}p_{ja}$	macTotProcTime					
ϕ_{11}	total work remaining for machine	$\sum_{j' \in \mathscr{J} \setminus \mathscr{J}_a} p_{j'a}$	macWrm					
ϕ_{12}	number of assigned operations for machine	$ \mathcal{J}_a $	macOps					
ϕ_{13}	change in idle time by assignment	$\Delta s(a,j)$	reducedSlack					
ϕ_{14}	total idle time for machine	$\sum_{j' \in \mathscr{J}_a} s(a, j')$	macSlack					
ϕ_{15}	total idle time for all machines	$\sum_{a' \in \mathscr{M}} \sum_{j' \in \mathscr{J}_{a'}} s(a', j')$	allSlack					
ϕ_{16}	current makespan	$\max_{(j',a')\in\mathscr{J}\times\mathscr{M}_{i'}}\{x_f(j',a')\}$	makespan					

to the partial schedule. Examples of these are dispatching the job with the most work remaining (MWR) or alternatively the least work remaining (LWR). A survey of more than 100 of such rules are presented in [23]. However, the reader is referred to an in-depth survey for simple or *single priority dispatching rule* (SDR) by [9]. The SDRs assign an index to each job in the job-list and is generally only based on a few attributes and simple mathematical operations.

Designing priority dispatching rules requires recognizing the important attributes of the partial schedules needed to create a good scheduling rule. These attributes attempt to grasp key features of the schedule being constructed. Which attributes are most important will necessarily depend on the objectives of the scheduling problem. Attributes used in this study applied for each possible operation are given in Table 1, where the set of machines already dispatched for J_j is $\mathcal{M}_j \subset \mathcal{M}$, and similarly, M_a has already had the jobs $\mathcal{J}_a \subset \mathcal{J}$ previously dispatched. The attributes of particular interest were obtained by inspecting the aforementioned SDRs. Attributes ϕ_1 - ϕ_8 and ϕ_9 - ϕ_{16} are job-related and machine-related, respectively. All of these attributes vary throughout the scheduling process, w.r.t. operation belonging to the same time step k, with the exception of ϕ_6 and ϕ_{10} which are static for a given problem instance but varying for each $J_j \in \mathcal{J}$ and $M_a \in \mathcal{M}$, respectively.

Priority dispatching rules are attractive since they are relatively easy to implement, fast and find good schedules. In addition, they are relatively easy to interpret, which makes them desirable for the end-user. However, they can also fail unpredictably. A careful combination of dispatching rules can perform significantly better [13]. These are referred to as *composite priority dispatching rules* (CDR), where the priority ranking is an expression of several single priority dispatching rules. CDRs deal with a greater number of features and more complicated form, in short, CDR is a combination of several SDRs. For instance let π be a CDR comprised of d DRs, then the index I for $J_i \in \mathcal{L}^{(k)}$ using π is,

$$I_j^{\pi} = \sum_{i=1}^d w_i \cdot \pi_i(\phi_j) \tag{9}$$

where $w_i > 0$ and $\sum_{i=0}^{d} w_i = 1$ with w_i giving the weight of the influence of π_i (which could be a SDR or another CDR) to π . Note, each π_i is function of J_j 's attributes ϕ_j . At each time step k, an operation is dispatched which has the highest priority. If there is a tie, some other priority measure is used. Generally the priority dispatching rules are static during the entire scheduling process, however, ties could also be broken randomly.

Investigating 11 SDRs for JSP, [17] created a pool of 33 CDRs that strongly outperformed the ones they were based on, by using multi-contextual functions based on either on job waiting time or machine idle time (similar to ϕ_5 and ϕ_{14} in Table 1), i.e., the CDRs are a combination of those two key attributes and then the SDRs. However, there are no combinations of the basic SDRs explored, only said two attributes. Similarly, using priority rules to combine 12 existing DRs from the literature, [34] had 48 CDR combinations, yielding 48 different models to implement and test. It is intuitive to get a boost in performance by introducing new CDRs, since where one DR might be failing, another could be excelling so combining them together should yield a better CDR. However, these approaches introduce fairly ad-hoc solutions and there is no guarantee the optimal combination of dispatching rules are found.

The composite priority dispatching rule presented in Eq. (9) can be considered as a special case of a the following general linear value function,

 $h(\boldsymbol{\chi}) = \sum_{i=1}^{d} w_i \phi_i(\boldsymbol{\chi}). \tag{10}$

where the job to be dispatched, J_{j^*} , corresponds to the one highest value, i.e.,

$$J_{j^*} = \underset{J_j \in \mathcal{L}}{\operatorname{argmax}} \ h(\boldsymbol{\phi}_j) \tag{11}$$

Similarly, single priority dispatching rules may be described by this linear model. For instance, let all $w_i = 0$, but with following exceptions: $w_1 = -1$ for SPT, $w_1 = +1$ for LPT, $w_7 = -1$ for LWR and $w_7 = +1$ for MWR. Generally the weights **w** are chosen by the designer or the rule apriori. A more attractive approach would be to learn these weights from problem examples directly. We will now investigate how this may be accomplished.

We break randomly? We do now!

Take one iteration over this paragraph with Helga – Better?

4 Learning Priority Dispatching Rules from Problem Instances

In this section we will describe issues that must be addresses when learning new priority dispatching rules. At the same time we will describe the experimental setup used in our experimental study. The issues that must be addressed are as follows. The problem instances used for learning and their optimal solutions. The reconstruction of the optimal solution using a priority dispatching rule. The construction of the training set used for learning. Finally, the machine learning procedure used must be decided.

Problem Instances

The class of problem instances used in our studies is the job-shop scheduling problem described in section 2. Each instance will have different processing times, machine ordering and dimensions. Each instance will therefore create different challenges for a priority dispatching rule. Dispatching rules learned will be customized for the problems used for their training. For real world application using historical data would be most appropriate. The aim would be to learn a dispatching rule that works well on average for a distribution of problem instances. To illustrate the performance difference of priority dispatching rules on different problem distributions, within the same class of problems, consider the following three cases.

Problem instances for JSP are generated stochastically by fixing the number of jobs and machines to ten. A discrete processing time is sampled independently from a discrete uniform distribution from the interval $I = [u_1, u_2]$, i.e., $\mathbf{p} \sim \mathcal{U}(u_1, u_2)$. The machine order is a random permutation of all of the machines in the job-shop Two different processing times distributions were explored, namely $\mathcal{P}_{j.rnd}^{n\times m}$ where I = [1,99] and $\mathcal{P}_{j.rndn}^{n\times m}$ where I = [45,55]. These instances are referred to as random and random-narrow, respectively.

Although in the case of $\mathcal{P}_{j.rnd}^{n\times m}$ this may be an excessively large range for the uniform distribution, it is however chosen in accordance with the literature [3] for creating synthesised $J||C_{\text{max}}$ problem instances. In addition, w.r.t. the machine ordering, one could look into a subset of JSP where the machines are partitioned into two (or more) sets, where all jobs must be processed on the machines from the first set (in some random order) before being processed on any machine in the second set, commonly denoted as $J|2\text{sets}|C_{\text{max}}$ problems, but as discussed in [30] this family of JSP is considered "hard" (w.r.t. relative error from best known solution) in comparison with the "easy" or "unchallenging" family with the general $J||C_{\text{max}}$ set-up.

For this study synthetic JSP and FSP problem instances will be considered with the problem size 10×10 . For each problem space N_{train} and N_{test} instances were generated for training and testing, respectively. Moreover, of the training data, 20% is reserved for validation. Summary of problem classes is given in Table 2. Note, that difficult problem instances are not filtered out beforehand, such as the approach in [32].

Problem instances for FSP are such that processing times are i.i.d. and uniformly distributed, $\mathscr{P}_{f.rnd}^{n\times m}$ where $\mathbf{p} \sim \mathscr{U}(1,99)$, referred to as random. In the JSP context $\mathscr{P}_{f.rnd}^{n\times m}$ is analogous to $\mathscr{P}_{j.rnd}^{n\times m}$.

use this somewhere else

Table 2 Problem space distributions used in experimental studies. Note, problem instances are synthetic and each problem space is i.i.d.

type	name	size $(n \times m)$	$N_{\rm train}$	N_{test}	note
JSP	$\mathcal{P}_{j.rnd}^{10\times10}$	10 × 10	300	200	random
	$\mathcal{P}_{j.rndn}^{10\times10}$	10 × 10	300	200	random-narrow
FSP	$\mathcal{P}_{f.rnd}^{10\times10}$	10×10	300	200	random

4.1 Comparing Operations

When building a complete schedule $\ell=n\cdot m$ dispatches must be made sequentially. A job is placed at the earliest available time slot for its next machine, whilst still fulfilling that each machine can handle at most one job at each time, and jobs need to have finished their previous machines according to its machine order. Unfinished jobs are dispatched one at a time according to some heuristic. After each dispatch the schedule's current features (cf. Table 1) are updated based on the half-finished schedule.

It is easy to see that the sequence of task assignments is by no means unique. Inspecting a partial schedule further along in the dispatching process such as in Fig. 1, then let's say J_1 would be dispatched next, and in the next iteration J_2 . Now this sequence would yield the same schedule as if J_2 would have been dispatched first and then J_1 in the next iteration, i.e., these are non-conflicting jobs. In this particular instance, one cannot infer that choosing J_1 is better and J_2 is worse (or vice versa) since they can both yield the same solution.

Note that in some cases there can be multiple optimal solutions to the same problem instance. Hence not only is the sequence representation 'flawed' in the sense that slight permutations on the sequence are in fact equivalent w.r.t. the end-result, but very varying permutations on the dispatching sequence (however given the same partial initial sequence) can result in very different complete schedules but can still achieve the same makespan, and thus same deviation from optimality, ρ , defined by Eq. (16), which is the measure under consideration. Care must be taken in this case that neither resulting features are labelled as undesirable. Only the resulting features from a dispatch resulting in a suboptimal solution should be labelled undesirable.

The optimum makespan is known for each problem instance. At each time step a number of feature pair are created, they consist of the features ϕ_o resulting from optimal dispatches $o \in \mathcal{O}^{(k)}$, versus features ϕ_s resulting from suboptimal dispatches $s \in \mathcal{S}^{(k)}$ at time k. In particular, each job is compared against another job of the joblist, $\mathcal{L}^{(k)}$, and if the makespan differs, i.e., $C_{\max}^{(s)} \geq C_{\max}^{(o)}$, an optimal/suboptimal pair is created, however if the makespans are identical the pair is omitted since they give the same optimal makespan. This way, only features from a dispatch resulting in a suboptimal solution is labelled undesirable.

Dispatch and time step are used interchangeably.

The approach taken here is to verify analytically, at each time step, by fixing the current temporal schedule as an initial state, whether it can indeed *somehow* yield an optimal schedule by manipulating the remainder of the sequence. This also takes care of the scenario that having dispatched a job resulting in a different temporal makespan would have resulted in the same final makespan if another optimal dispatching sequence would have been chosen. That is to say the data generation takes into consideration when there are multiple optimal solutions to the same problem instance.

4.2 Generating Training Data

Preliminary experiments for creating step-by-step model was done in [10] where an optimal trajectory was explored, i.e., at each dispatch some (random) optimal task is dispatched, resulting in local linear model for each dispatch; a total of ℓ linear models for solving $n \times m$ JSP. However, the experiments there showed that by fixing the weights to its mean value throughout the dispatching sequence, results remained satisfactory. A more sophisticated way, would be to create a new linear model, where the preference set, S, is the union of the preference pairs across the ℓ dispatches. This would amount to a substantial preference set, and for S to be computationally feasible to learn, S has to be reduced. For this several ranking strategies were explored in [11], the results there showed that it's sufficient to use partial subsequent rankings, namely, combinations of r_i and r_{i+1} for $i \in \{1, ..., n'\}$, are added to the preference set, where $r_1 > r_2 > ... > r_{n'}$ $(n' \le n)$ are the rankings of the job-list, $\mathcal{L}^{(k)}$, at time step k, in such a manner that in the cases that there are more than one operation with the same ranking, only one of that rank is needed to be compared to the subsequent rank. Moreover, in the case of this study, which deals with 10×10 problem instances, the partial subsequent ranking becomes necessary, as full ranking is computationally infeasible. This is due to the fact the size of the preference set, |S|, becomes too large with full ranking, and would need sampling. For the following experimental set up, the preference set was limited to $|S| \le 500,000$ by random sampling.

4.3 Linear Learning

Learning models considered in this study are based on ordinal regression in which the learning task is formulated as learning preferences. In the case of scheduling, learning which operations are preferred to others. Ordinal regression has been previously presented in [28] and in [10] for JSP, however given here for completeness.

Let $\phi_o \in \mathbb{R}^d$ denote the post-decision state when dispatching J_o corresponds to an optimal schedule being built. All post-decisions states corresponding to suboptimal dispatches, J_s , are denoted by $\phi_s \in \mathbb{R}^d$. One could label which feature sets were considered optimal, $\mathbf{z}_o = \phi_o - \phi_s$, and suboptimal, $\mathbf{z}_s = \phi_s - \phi_o$ by $y_o = +1$ and $y_s = -1$ respectively. Note, a negative example is only created as long as J_s actually results in a worse makespan, i.e., $C_{\max}^{(s)} \geq C_{\max}^{(o)}$, since there can exist situations in which more than one operation can be considered optimal.

The preference learning problem is specified by a set of preference pairs,

$$S = \left\{ \left(\mathbf{z}_{o}, +1\right), \left(\mathbf{z}_{s}, -1\right) \mid \forall (o, s) \in \mathcal{O}^{(k)} \times \mathcal{S}^{(k)} \right\}_{k=1}^{\ell} \subset \mathbf{\Phi} \times Y$$
 (12)

where $\Phi \subset \mathbb{R}^d$ is the training set of d features, $Y = \{-1, +1\}$ is the outcome space, $\ell = n \times m$ is the total number dispatches, from which $o \in \mathcal{O}^{(k)}$ and $s \in \mathcal{S}^{(k)}$ denote optimal and suboptimal dispatches, respectively, at step k. Note, $\mathcal{O}^{(k)} \cup \mathcal{S}^{(k)} = \mathcal{L}^{(k)}$, and $\mathcal{O}^{(k)} \cap \mathcal{S}^{(k)} = \emptyset$.

For JSP there are d = 16 features (cf. Table 1 and explained in more detail in ??), and the training set is created in the manner described in Section 4.

Now consider the model space $\mathscr{H} = \{h(\cdot) : X \mapsto Y\}$ of mappings from solutions to ranks. Each such function h induces an ordering \succ on the solutions by the following rule,

$$\mathbf{x}_i \succ \mathbf{x}_j \quad \Leftrightarrow \quad h(\mathbf{x}_i) > h(\mathbf{x}_j)$$
 (13)

where the symbol \succ denotes "is preferred to." The function used to induce the preference is defined by a linear function in the feature space,

$$h(\mathbf{x}) = \sum_{i=1}^{d} w_i \phi_i(\mathbf{x}) = \langle \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}) \rangle.$$
 (14)

Logistic regression learns the optimal parameters $\mathbf{w}^* \in \mathbb{R}^d$. For this study, L2-regularized logistic regression from the LIBLINEAR package [4] without bias is used to learn the preference set S, defined by Eq. (12). Hence, for each job on the job-list, $J_j \in \mathcal{L}$, let ϕ_j denote its corresponding post-decision state. Then the job chosen to be dispatched, J_{j^*} , is the one corresponding to the highest preference estimate, i.e.,

$$J_{j^*} = \underset{J_i \in \mathscr{L}}{\operatorname{argmax}} \ h(\boldsymbol{\phi}_j) \tag{15}$$

where $h(\cdot)$ is the classification model obtained by the preference set.

4.4 Interpreting linear classification models

Looking at the features description in Table 1 it is possible for the ordinal regression to 'discover' the weights **w** in order for Eq. (14) corresponds to applying a single priority dispatching rules from ??. For instance,

$$SPT: w_i = \begin{cases} -1 \text{ if } i = 1\\ 0 \text{ otherwise} \end{cases}$$

$$LPT: w_i = \begin{cases} +1 \text{ if } i = 1\\ 0 \text{ otherwise} \end{cases}$$

$$MWR: w_i = \begin{cases} +1 \text{ if } i = 7\\ 0 \text{ otherwise} \end{cases}$$

$$LWR: w_i = \begin{cases} -1 \text{ if } i = 7\\ 0 \text{ otherwise} \end{cases}$$

where $i \in \{1, ..., d\}$. When using a feature space based on SDRs, the linear classification models can very easily be interpreted as CDRs with predetermined weights.

The goal is to minimize the makespan, C_{max} . The optimum makespan is denoted $C_{\text{max}}^{\text{opt}}$, and the makespan obtained from the scheduling policy A under inspection by C_{max}^A . Since the optimal makespan varies between problem instances the performance measure is the following,

$$\rho = \frac{C_{\text{max}}^A - C_{\text{max}}^{\text{opt}}}{C_{\text{max}}^{\text{opt}}} \cdot 100\%$$
 (16)

which indicates the percentage relative deviation from optimality.

5 Performance of SDR

In order to create successful dispatching rules, a good starting point is to investigate the properties of optimal solutions and hopefully be able to learn how to mimic such "good" behaviour. For this, we follow an optimal solution, obtained by using a commercial software package [8], and inspect the evolution of its features, defined in Table 1. Moreover, it is noted, that there are several optimal solutions available for each problem instance. However, it is deemed sufficient to inspect only one optimal trajectory per problem instance as there are $N_{\text{train}} = 300$ independent instances which gives the training data variety.

5.1 Probability of choosing optimal decision

Firstly, we can observe that on a step-by-step basis there are several optimal dispatches to choose from. Figure 2 depicts how the number of optimal dispatches evolve at each dispatch iteration. Note, that only one optimal trajectory is pursued (chosen at random), hence this is only a lower bound of uniqueness of optimal solutions. As the number of possible dispatches decrease over time, Fig. 3 depicts the probability of choosing an optimal dispatch.

5.2 Making suboptimal decisions

Looking at Fig. 3, $\mathcal{P}_{j,rnd}^{10\times 10}$ has a relatively high probability (70% and above) of choosing an optimal job. However, it is imperative to keep making optimal decisions, because once off the optimal track the consequences can be dire. To demonstrate this Fig. 4 depicts mean worst and best case scenario of the resulting deviation from optimality, ρ , once you've fallen off the optimal track. Note, that this is given that you make *one* wrong turn. Generally, there will be more, and then the compound effects of making suboptimal decisions really start adding up.

It is interesting that for JSP, that over time making suboptimal decisions make more of an impact on the resulting makespan. This is most likely due to the fact that if suboptimal decision is made in the early stages, then there is space to rectify the

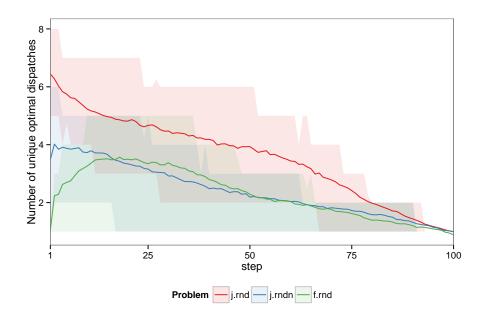
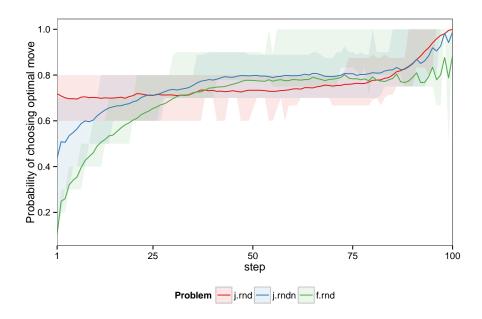


Fig. 2 Number of unique optimal dispatches (lower bound)



 $\textbf{Fig. 3} \ \ \text{Probability of choosing optimal move}$

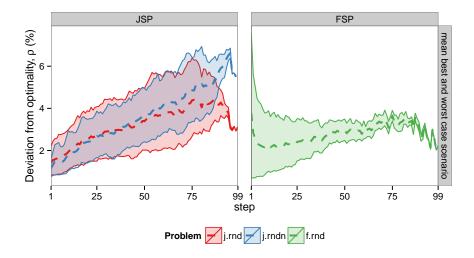


Fig. 4 Mean deviation from optimality, ρ , (%), for best (lower bound) and worst (upper bound) case scenario of choosing suboptimal dispatch for $\mathscr{P}_{j.rnd}^{10\times 10}$, $\mathscr{P}_{j.rndn}^{10\times 10}$ and $\mathscr{P}_{f.rnd}^{10\times 10}$

situation with the subsequent dispatches. However, if done at a later point in time, little is to be done as the damage is already inflicted upon the schedule. However, for FSP, the case is the exact opposite. Then it's imperative to make good decisions right from the beginning. This is due to the major structural differences between JSP and FSP, namely the latter having a homogeneous machine ordering, constricting the solution immensely. Luckily, this does have the added benefit of making it less vulnerable for suboptimal decisions later in the decision process.

5.3 Optimality of single priority dispatching rules

The probability of optimality of the aforementioned SDRs from ??, yet still maintaining our optimal trajectory, i.e., the probability of a job chosen by a SDR being able to yield an optimal makespan on a step-by-step basis, is depicted in Fig. 5. Moreover, the dashed line represents the benchmark of random guessing (cf. Fig. 3).

Now, let's bare in mind the deviation from optimality of applying SDRs throughout the dispatching process (box-plots of which are depicted in Fig. 6) then there is a some correspondence between high probability of stepwise optimality and low ρ . Alas, this isn't always the case, for $\mathcal{P}_{j.rnd}^{10\times 10}$, SPT always outperforms LPT w.r.t. stepwise optimality, however this does not transcend to SPT having a lower ρ value than LPT. Hence, it's not enough to just learn optimal behaviour, one needs to investigate what happens once we encounter suboptimal state spaces.

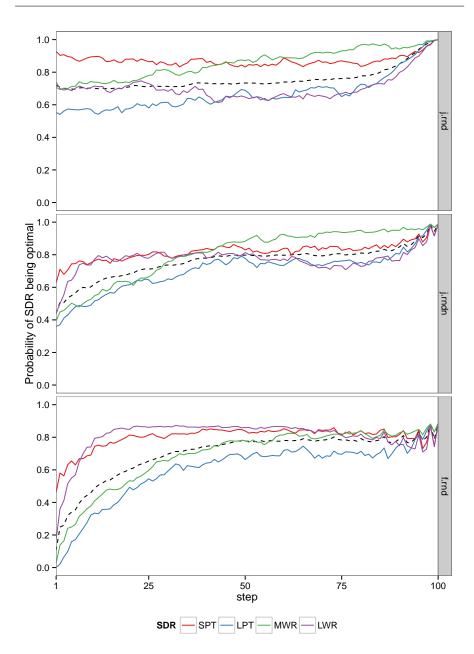


Fig. 5 Probability of SDR being optimal

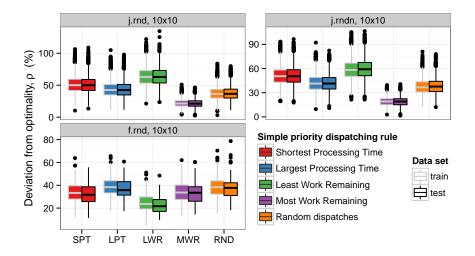


Fig. 6 Box plot for deviation from optimality, ρ , (%) for SDRs

5.4 Simple blended dispatching rule

A naive approach to create a simple blended dispatching rule would be for instance be switching between two SDRs at a predetermined time point. Hence, going back to Fig. 5 a presumably good BDR for $\mathcal{P}_{j,rnd}^{10\times10}$ would be starting with SPT and then switching over to MWR at around time step 40, where the SDRs change places in outperforming one another. A box-plot for ρ for all problem spaces is depicted in Fig. 7. Now, this little manipulation between SDRs does outperform SPT immensely, yet doesn't manage to gain the performance edge of MWR, save for $\mathcal{P}_{f,rnd}^{10\times10}$. This gives us insight that for job-shop based problem spaces, the attribute based on MWR is quite fruitful for good dispatches, whereas the same cannot be said about SPT – a more sophisticated BDR is needed to improve upon MWR.

A reason for this lack of performance of our proposed BDR is perhaps that by starting out with SPT in the beginning, it sets up the schedules in such a way that it's quite greedy and only takes into consideration jobs with shortest immediate processing times. Now, even though it is possible to find optimal schedules from this scenario, as Fig. 5 show, the inherent structure that's already taking place, and might make it hard to come across by simple methods. Therefore it's by no means guaranteed that by simply swapping over to MWR will handle that situation which applying SPT has already created. Figure 7 does however show, that by applying MWR instead of SPT in the latter stages, does help the schedule to be more compact w.r.t. SPT. However, in the case of $\mathcal{P}_{j,rnd}^{10\times10}$ and $\mathcal{P}_{j,rndn}^{10\times10}$ the fact remains that the schedules have diverged too far from what MWR would have been able to achieve on its own. Preferably the blended dispatching rule should use best of both worlds, and outperform all of its inherited DRs, otherwise it goes without saying one would simply still use the original DR that achieved the best results.

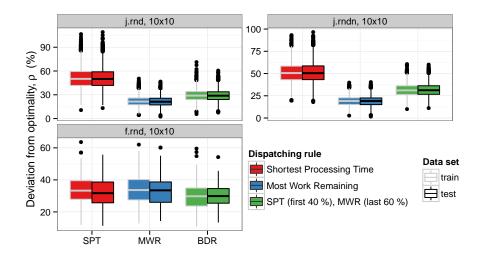


Fig. 7 Box plot for deviation from optimality, ρ , (%) for BDR where SPT is applied for the first 40% of the dispatches, followed by MWR

6 Learning CDR

Section 5.4 demonstrates there is definitely something to be gained by trying out different combinations, it's just non-trivial how to go about it, and motivates how it's best to go about learning such interaction, which will be addressed in this section.

6.1 Feature Selection

The SDRs we've inspected so-far are based on two features from Table 1, namely

- ϕ_1 for SPT and LPT
- $-\phi_7$ for LWR and MWR

by choosing the lowest value for the first SDR, and highest value for the latter SDR, i.e., the extremal values for those given features. There is nothing that limits us to using just those two features.

For this study we will consider all combinations of features using either one, two, three or all of the features, for a total of $\binom{d}{1} + \binom{d}{2} + \binom{d}{3} + \binom{d}{d}$, i.e., total of 697 combinations. The reason for such a limiting number of active features, are due to the fact we want to keep the models simple enough for improved model interpretability

 $^{^2\,}$ Software available at http://www.csie.ntu.edu.tw/~cjlin/liblinear

in Section 4. Note, in order to report the validation accuracy, 20% (N = 60) of the training set was set aside for validation of reporting the accuracy.

6.2 Validation accuracy

As the preference set *S* has both preference pairs belonging to optimal ranking, and subsequent rankings, it is not of primary importance to classify *all* rankings correctly, just the optimal ones. Therefore, instead of reporting the validation accuracy based on the classification problem of the correctly labelling the problem set *S*, it's opted the validation accuracy is obtained in the same manner as done in Section 5.3 for SDRs, i.e., the probability of choosing optimal decision given the resulting linear weights, however in this context, the mean throughout the dispatching process is reported. Figure 8 shows the difference between the two measures of reporting validation accuracy. Validation accuracy based on stepwise optimality only takes into consideration the likelihood of choosing the optimal move at each time step. However, the classification accuracy is also trying to correctly distinguish all subsequent rankings in addition of choosing the optimal move, as expected that measure is considerably lower.

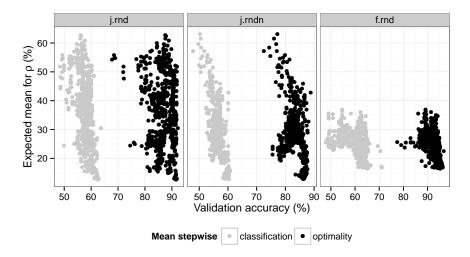


Fig. 8 Various methods of reporting validation accuracy for preference learning

6.3 Pareto front

When training the learning model one wants to keep the validation accuracy high, as that would imply a higher likelihood of making optimal decisions, which would in turn translate into a low final makespan. To test the validity of this assumptions, each of the 697 models is run on the preference set, and its mean ρ is reported against its corresponding validation accuracy in Fig. 9. The models are colour-coded w.r.t. the number of active features, and a line is drawn through its Pareto front. Moreover, those solutions are labelled with their corresponding model ID. Moreover, the Pareto front over all 697 models, irrespective of active feature count, is denoted with triangles. Moreover, their values are reported in Table 3, where the best objective is given in boldface.

Section 4.4 showed how to interpret the linear preference models by their weights. Figure 10 depicts the linear weights, \mathbf{w} , from Eq. (13) for all of the CDR models reported in Table 3. The weights have been normalised for clarity purposes, such that it is scaled to $\|\mathbf{w}\| = 1$, thereby giving each feature their proportional contribution to the preference I_j^{π} defined by Eq. (9). These weights will now be explored further, along with testing whether models are statistically significant to one another, using a Kolmogorov-Smirnov test with $\alpha = 0.05$.

For $\mathscr{P}_{j,rnd}^{10\times 10}$ there is no statistical difference between models (2.69, 3.355, 3.358, 3.524), w.r.t. ρ and the latter three w.r.t. accuracy. These models are therefore equivalently 'best' for the problem space. As Fig. 10 shows, ϕ_3 , ϕ_7 and ϕ_{11} are similar in value, and in the case of 3.358, then ϕ_9 has similar contribution as ϕ_3 for the other models. Which, as standalone models are 1.6 and 1.3, respectively, and yield equivalent mean ρ and accuracy. As these features often coincide in job-shop it is justifiable to use only either one, as the it contains the same information as its counterpart. Most likely, the equivalence of these features is indicating that the schedules are rarely able to dispatch in earlier slots, i.e., $\phi_3 \equiv \phi_9$.

In addition, (2.111, 3.300) and (16.1, 3.355) are statistically insignificant w.r.t. validation accuracy for $\mathcal{P}_{j.rnd}^{10\times 10}$. However, they have considerable performance difference w.r.t. ρ ($\Delta \rho \approx 18\%$). So even looking at stepwise optimality by itself is very fickle, because slight variations can be quite dramatic to the end result.

The solutions on the Pareto front for $\mathcal{P}_{j.rndn}^{10\times10}$ are quite a few models with no (or minimal) statistical difference w.r.t. ρ , and considerably more w.r.t. validation accuracy. Most notably are (3.281, 2.73, 2.75, 1.13), (note, first one has the lowest mean ρ) which are all statistically insignificant w.r.t. validation accuracy yet none w.r.t. ρ , with difference up to $\Delta \rho = 6.32\%$.

For $\mathscr{P}_{f.rnd}^{10\times10}$ almost all models are statistically different w.r.t. ρ , only exception is (1.6, 1.7). Although, w.r.t. validation accuracy, there are a few equivalent models, namely, (3.151, 2.51), (2.94, 1.6) and (3.216, 3.213, 16.1), with 1.2%, 2.3% and 5.75% difference in mean ρ , respectively.

It's interesting to inspect the full model for $\mathscr{P}_{f.rnd}^{10\times 10}$, 16.1. Despite having similar contributions, yet statistically significantly different, as all the active features as (3.213, 3.216), then the (slight) interference from of other features, hinders the full model from achieving a low ρ . Only considering ϕ_8 and ϕ_{12} with either ϕ_3 and ϕ_9 , boosts performance by 5.28% and 5.72%, respectively. Thereby stressing the importance of feature selection, to steer clear of over-fitting. Note, unlike $\mathscr{P}_{i.rnd}^{10\times 10}$, now ϕ_3

³ Note, $\phi_3 \le \phi_9$, where $\phi_3 = \phi_9$ when J_j is the latest job on M_a , otherwise J_j is placed in a previously created slot on M_a .

Table 3 Mean validation accuracy and mean expected deviation from optimality, ρ , for all CDR models on the Pareto from Fig. 9.

Problem	PREF	Accuracy (%)		ρ (%)	Pareto
	NrFeat.Model	Optimality	Classification		
	3.524	91.55	62.57	12.67	A
	3.358	91.82	62.74	12.90	A
	3.355	91.90	62.71	12.92	A
	2.69	91.02	61.41	12.92	
	1.11	80.77	55.78	21.63	
$\mathcal{P}_{j.rnd}^{10\times10}$	1.13	85.26	57.17	22.79	
J	16.1	92.24	63.61	30.47	A
	2.111	91.52	59.69	32.68	
	1.6	89.85	58.33	33.08	
	1.3	89.86	58.34	33.41	
	3.300	91.91	60.05	51.87	
	3.281	86.24	60.34	12.89	A
	3.231	86.52	58.92	12.98	A
	3.222	86.69	58.86	13.23	A
	2.68	86.19	59.27	13.34	
	3.223	86.73	58.80	13.44	A
	3.528	86.84	59.49	13.61	A
	2.52	86.47	59.16	13.65	
	2.73	86.55	59.26	13.67	
	3.159	86.88	58.87	13.91	A
	3.263	86.95	59.20	14.06	A
$\mathcal{P}_{j.rndn}^{10\times10}$	3.162	86.92	58.97	14.06	A
	2.51	86.65	58.90	14.06	
	3.147	87.18	58.88	14.29	A
	3.148	87.45	59.24	14.79	A
	2.75	87.11	60.45	15.30	
	3.418	87.75	59.57	16.22	A
	1.13	86.22	58.04	19.21	
	2.91	87.12	60.17	19.48	
	3.139	87.81	59.09	29.00	A
	3.237	88.07	59.40	32.69	A
	16.1	88.86	60.17	42.88	A
	3.539	95.22	64.97	16.40	A
	3.151	96.06	64.31	16.75	A
	3.216	96.28	71.12	16.78	A
	2.94	92.79	63.12	16.88	
$\mathcal{P}_{c}^{10\times10}$	3.213	96.30	71.05	17.22	A
f.rnd	2.111	94.16	65.07	17.73	
	2.51	95.83	64.21	17.95	
	1.7	87.59	61.74	19.05	
	1.6	92.61	62.91	19.18	
	16.1	96.67	70.58	22.50	A

differs from ϕ_9 , indicating that there are some slots created, which could be better utilised. Moreover, looking at model 2.111 for $\mathscr{P}_{f.rnd}^{10\times 10}$, which has similar contributions as the best model, 3.539. Then introducing a third feature, ϕ_{11} , is the key to the success of the CDR, with a boost of ρ performance by 1.33%.

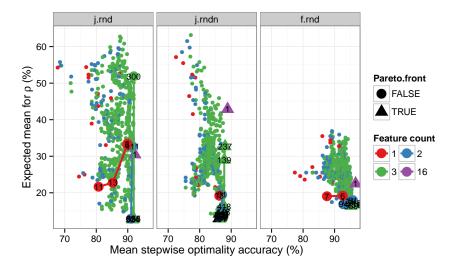


Fig. 9 Scatter plot for validation accuracy (%) against its corresponding mean expected ρ (%) for all 697 linear models, based on either one, two, three or all d combinations of features. Pareto fronts for each active feature count based on maximum validation accuracy and minimum mean expected ρ (%), and labelled with their model ID. Moreover, actual Pareto front over all models is marked with triangles.

Note, for both $\mathcal{P}_{j,rnd}^{10\times10}$ and $\mathcal{P}_{j,rndn}^{10\times10}$, model 1.13 is on the Pareto front. The model corresponds to feature ϕ_7 , and in both cases has a weight strictly greater than zero (cf. Fig. 10). Revisiting Section 4.4, we observe that this implies the learning model was able to discover MWR as one of the Pareto solutions, and as is expected, there is no statistical difference to between 1.13 and MWR.

As one can see from Fig. 9, adding additional features to express the linear model boosts performance in both validation accuracy and expected mean for ρ , i.e., the Pareto fronts are cascading towards more desirable outcome with higher number of active features. However, there is a cut-off point for such improvement, as using all features is generally considerably worse off due to overfitting of classifying the preference set.

Now, let's inspect the models corresponding to the minimum mean ρ and highest mean validation accuracy, highlighted in Table 3 and inspect the stepwise optimality for those models in Fig. 11, again using probability of randomly guessing an optimal move from Section 5.1 as a benchmark. As one can see for both $\mathcal{P}_{j,rndn}^{10\times 10}$ and $\mathcal{P}_{j,rndn}^{10\times 10}$, despite having a higher mean validation accuracy overall, the probabilities vary significantly. A lower mean ρ is obtained when the validation accuracy is gradually increasing over time, and especially during the last phase of the scheduling. A Revisiting Fig. 4, this trend indicates that it's likelier for the resulting makespan to be considerably worse off if suboptimal moves are made at later stages, than at earlier stages. Therefore, it's imperative to make the 'best' decision at the 'right' moment, not just

⁴ It's almost illegible to notice this shift directly from Fig. 11, as the difference between the two best models is oscillating up to only 3% at any given step. In fact $\mathscr{P}_{j,rdn}^{10\times 10}$ has the most clear difference w.r.t. classification accuracy of indicating when a minimum ρ model excels at choosing the preferred move.

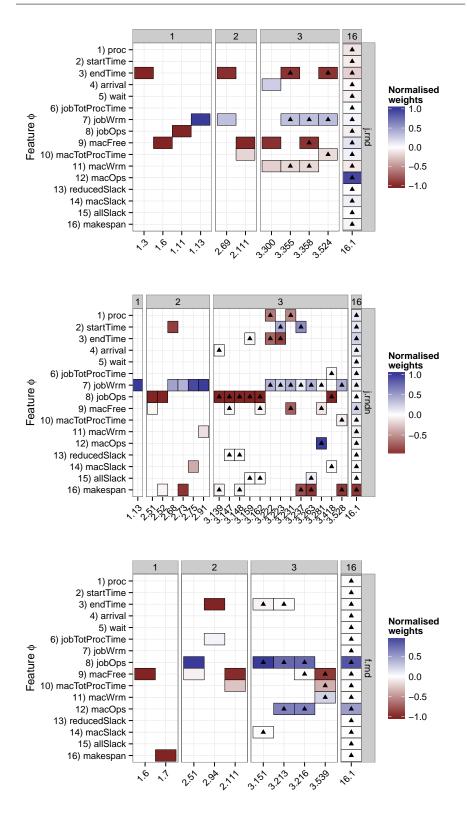


Fig. 10 Normalised weights for CDR models from Table 3, models are grouped w.r.t. its dimensionality, *d*. Note, a triangle indicates a solution on the Pareto front.

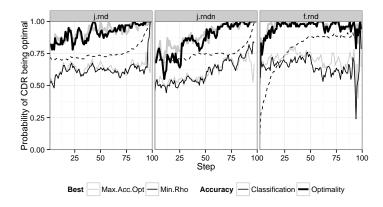


Fig. 11 Probability of choosing optimal move for models corresponding to highest mean validation accuracy (grey) and lowest mean deviation from optimality, ρ , (black) compared to the baseline of probability of choosing an optimal move at random (dashed).

look at the overall mean performance. Hence, the measure of validation accuracy as discussed in Section 6.2 should take into consideration the impact a suboptimal move yields on a step-by-step basis, e.g., weighted w.r.t. a curve such as depicted in Fig. 4.

Let's revert back to the original SDRs discussed in Section 5.3 and compare the best CDR models, a box-plot for ρ is depicted in Fig. 12. Firstly, there is a statistical difference between all models, and clearly the CDR model corresponding to minimum mean ρ value, is the clear winner, and outperforms the SDRs substantially. However, the best model w.r.t. maximum validation accuracy, then the CDR model shows a lacklustre performance. In some cases it's better off, e.g., compared to LWR, yet for job-shop it doesn't surpass the performance of MWR. This implies, the learning model is over-fitting the training data. Results hold for the test set.

7 Conclusions

Current literature still hold single priority dispatching rules in high regard, as they are simple to implement and quite efficient. However, they are generally taken for granted as there is clear lack of investigation of *how* these dispatching rules actually work, and what makes them so successful (or in some cases unsuccessful)? For instance, of the four SDRs this study focuses on, why does MWR outperform so significantly for jobshop yet completely fail for flow-shop? MWR seems to be able to adapt to varying distributions of processing times, however manipulating the machine ordering causes MWR to break down. By inspecting optimal schedules, and meticulously researching what's going on, every step of the way of the dispatching sequence, some light is shed where these SDRs vary w.r.t. the problem space at hand. Once these simple rules are understood, then it's feasible to extrapolate the knowledge gained and create new composite priority dispatching rules that are likely to be successful.

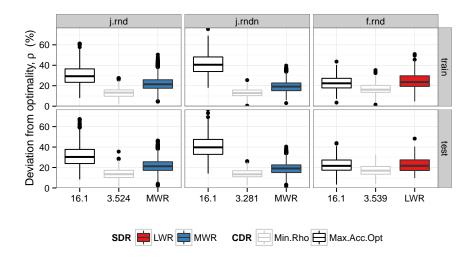


Fig. 12 Box plot for deviation from optimality, ρ , (%) for the best CDR models (cf. Table 3) and compared against the best SDRs from Section 5.3, both for training and test sets.

Creating new dispatching rules is by no means trivial. For job-shop there is the hidden interaction between processing times and machine ordering that's hard to measure. Due to this artefact, feature selection is of paramount importance, and then it becomes the case of not having too many features, as they are likely to hinder generalisation due to over-fitting in training. However, the features need to be explanatory enough to maintain predictive ability. For this reason Section 6 was limited to up to three active features, as the full feature set was clearly sub-optimal w.r.t. the SDRs used as a benchmark. By using features based on the SDRs, along with some additional local features describing the current schedule, it was possible to 'discover' the SDRs when given only one active feature. Furthermore, by adding on additional features, a boost in performance was gained, resulting in a composite priority dispatching rule that outperformed all of the SDR baseline.

When training the learning model, it's not sufficient to only optimize w.r.t. highest mean validation accuracy. As Section 6.3 showed, there is a trade-off between making the over-all best decisions versus making the right decision on crucial time points in the scheduling process, as Fig. 4 clearly illustrated. It is for this reason, traditional feature selection such as add1 and drop1 were unsuccessful in preliminary experiments, and thus resorting to having to exhaustively search all feature combinations. This also opens of the question of how should validation accuracy be measured? Since the model is based on learning preferences, both based on optimal versus suboptimal, and then varying degrees of sub-optimality. As we are only looking at the ranks in a black and white fashion, such that the makespans need to be strictly greater to belong to a higher rank, then it can be argued that some ranks should be grouped together if their makespans are sufficiently close. This would simplify the training set, making it (presumably) less of contradictions and more appropriate for linear learning. Or

simply the validation accuracy could be weighted w.r.t. the difference in makespan. During the dispatching process, there are some pivotal times which need to be especially taken care off. Figure 4 showed how making suboptimal decisions were more of a factor during the later stages, whereas for flow-shop the case was exact opposite.

Could discuss new sampling strategies, e.g., proportional to best/worst case, optimality, etc. – have done some experiments, but not clear what strategy is best, so only equal probability reported

Despite the abundance of information gathered by following an optimal trajectory, the knowledge obtained is not enough by itself. Since the learning model isn't perfect, it is bound to make a mistake eventually. When it does, the model is in uncharted territory as there is not certainty the samples already collected are able to explain the current situation. For this we propose investigating features from suboptimal trajectories as well, since the future observations depend on previous predictions. A straight forward approach would be to inspect the trajectories of promising SDRs or CDRs. In fact, it would be worth while to try out imitation learning by [26,27], such that the learned policy following an optimal trajectory is used to collect training data, and the learned model is updated. This can be done over several iterations, with the benefit being, that the states that are likely to occur in practice are investigated, and as such used to dissuade the model from making poor choices. Alas, this comes at great computational cost due to the substantial amounts of states that need to be optimised for their correct labelling. Making it only practical for job-shop of a considerable lower dimension.

Although this study has been structured around the job-shop scheduling problem, it is easily extended to other types of deterministic optimisation problems that involve sequential decision making. The framework presented here collects snap-shots of the state space by following an optimal trajectory, and verifying the resulting optimal makespan from each possible state. From which the stepwise optimality of individual features can be inspected, which could for instance justify omittance in feature selection. Moreover, by looking at the best and worst case scenario of suboptimal dispatches, it is possible to pinpoint vulnerable times in the scheduling process.

Not done, but possible

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