Ranking and Selection: A New Sequential Bayesian Procedure for Use with Common Random Numbers

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October 27, 2014

Abstract

We want to select the best systems out of a given set of systems (or rank them) with respect to their expected performance. The systems allow random observations only and we assume that the joint observation of the systems has a multivariate normal distribution with unknown mean and covariance. We allow dependent marginal observations as they occur when common random numbers are used for the simulation of the systems. In particular, we focus on positively dependent observations as they might be expected in heuristic optimization where 'systems' are different solutions to an optimization problem with common random inputs.

In each iteration, we allocate a fixed budget of simulation runs to the solutions. We use a Bayesian setup and allocate the simulation effort according to the posterior covariances of the solutions until the ranking and selection decision is correct with a given high probability. Here, the complex posterior distributions are approximated only but we give extensive empirical evidence that the observed error probabilities are well below the given bounds in most cases.

We also use a generalized scheme for the target of the ranking and selection that allows to bound the error probabilities with a Bonferroni approach. Our test results show that our procedure uses less simulations than comparable procedures from literature even in most of the cases where the observations are not positively correlated.

keywords: Sequential Ranking and Selection, Common Random Numbers, Bayesian Statistics, Multiple Testing, Missing Data

1 Introduction

We consider ranking and selection of systems based on the average performance of the alternatives. The particular set-up used here is motivated by problems

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from optimization under uncertainty.

Often in operations research as well as in technical applications the performance of solutions depends on some random influence like market conditions, material quality, or simply measurement errors. We shall call such random influences a random *scenario*. Usually, the aim is then to find a solution with minimal expected costs taken over all scenarios. We assume here that we can describe the random scenario mathematically by a random variable Z with a distribution $\mathbf{P}_Z$. Let $c(s, z)$ denote the cost of solution s if it has been applied to random scenario z, then the average costs are given by the expectation $\mathbf{E}c(s, Z)$. Except for particularly simple cases, we will not be able to calculate this expression analytically. Instead, we have to estimate $\mathbf{E}c(s, Z)$ based on a sample $c(s, z_1), \ldots, c(s, z_n)$, where $z_1, \ldots, z_n$ are observations of the random variable Z, usually produced by a stochastic simulation model on a computer.

With estimated costs, optimization can be performed by heuristic search methods like genetic algorithms or ant algorithms. Typically, these methods take a relatively small set $\mathcal{L} := \{s_1, \ldots, s_L\}$ of solutions (a 'population') and try to improve the quality of $\mathcal{L}$ iteratively. The improvement step usually includes a *selection* of the best or at least the most promising solutions from $\mathcal{L}$ with respect to their expected costs $\mu_i := \mathbf{E}c(s_i, Z)$. As μ_i can only be estimated, this selection will return sub-optimal solutions with a certain error probability. Often, this probability can be made arbitrarily small by increasing the sample size n, i.e. the number of simulations.

The aim of this paper is to find selection mechanisms for good solutions suitable for heuristic optimization that have error probabilities below a given bound and use few simulations only.

Most heuristic optimization procedures do not need the exact values of $\mu_1, \ldots, \mu_L$ in order to perform a reasonable selection, instead it is sufficient to find the correct *ranking* $\mu_{i_1} \leq \cdots \leq \mu_{i_L}$ or even only part of it. As it has been noted before (see e.g. Xie [1995]) it is much easier (needs less simulations) to estimate the correct ranking than to estimate the correct values. Methods of ranking and selection are therefore widely used in heuristic optimization under uncertainty, see e.g. Schmidt et al. [2006] for an overview.

In this paper we have a fixed set $\mathcal{L} = \{1, \ldots, L\}$ of solutions, the observed cost values are assumed to be normally distributed with unknown mean and unknown covariance matrix. We use a Bayesian approach and estimate the ranks of the solutions in each iteration based on the present posterior means. Roughly, the steps of our procedure to rank and select the solutions can be summarized as follows:

1. Initialization: observe all solutions for a fixed number n_0 of scenarios (=simulations).

2. Determine the ranking and selection based on the posterior means given these observations.

3. Calculate a lower bound LB(PCS) for the *probability of correct selection* PCS

4. While LB(PCS) $< 1 - \alpha$ do
   (a) allocate a fixed *budget* of additional simulations to the solutions,
   (b) recalculate the posterior means, the ranking and selection and LB(PCS) based on the extended set of observations.
5. Return the last ranking and selection.

Input parameters are the allowed error probability α, the simulation budget b and the initial sample size n_0.

This is the standard framework of a (Bayesian) computing budget allocation (CBA) algorithm, see e.g. in Chen and Lee [2010]. Our contributions concern the following points which we label for further reference:

Depend We allow for *dependent observations*, i.e. we apply the solutions to common random scenarios (common random numbers, CRN) observing $(c(1, Z), \ldots, c(L, Z))$, a vector of possibly dependent, normally distributed values.

Target We use a very *general concept of a target* for ranking and selection that includes targets as median or span of means and still allows to bound the probability of a correct selection in a simple Bonferroni fashion.

Alloc Most importantly, we introduce a new *heuristic allocation scheme* for additional simulations based on the posterior distribution of the means and the covariance matrix. This scheme reuses terms that have been evaluated to calculate the LB(PCS) in the iteration before and therefore requires little additional effort. In the experiments described below, our algorithm needed less simulations to guarantee LB(PCS)$\geq 1 - \alpha$ than competitors from literature.

Let us discuss these issues in more detail.

Depend: Classical ranking and selection (R&S) procedures evaluate the alternatives based on random scenarios drawn *independently* for each alternative , see e.g. Kim and Nelson [2006a]. Only a few authors (see e.g. Chick and Inoue [2001]) use *dependent* samples based on common random numbers (CRN) for simulation. It is well known, that if the observations are *positively correlated*, it is more efficient to use common random numbers (CRN), i.e. to compare the solutions on the same scenario (see e.g. Glasserman and Yao [1992]). Positive correlation in our case roughly means that if a solution $s \in \mathcal{L}$ has, for a scenario z, costs $c(s, z)$ that are above average, then costs $c(s', z)$ will tend to be over average for all the other solutions $s' \in \mathcal{L}$ also. In other words, if some scenario z is relatively difficult (costly) for solution s, then z will tend to be difficult for all solutions. Similarly, a scenario that has small costs (below average) for one solution will tend to be an easy scenario for all solutions creating smaller costs for all of them.

As this is the behaviour we would expect from a set of solutions at least after some iterations of improvement, it seems to be justified to expect positive

correlation and to use CRN specific R&S procedures for heuristic optimization. The numerical results below show that if the cost are positively correlated huge savings in simulation effort are indeed possible and if there is no positive correlation our approach is not worse than other procedures.

Target: We fix a set $A \subset \{1, , \ldots, L\}$ of ranks and try to select (only) those solutions that have these ranks with respect to the posterior means (and sort them if necessary). E.g. if we have $A := \{1, \ldots, k\}$ then we want to select the k best solutions (with minimal means). We describe the sets of possible correct selections in a way that uses a minimal set of pairwise comparisons of solutions, see Schmidt et al. [2006] for a similar approach. This allows to give a Bonferroni type of lower bound to the posterior probability of correct selection that involve only one-dimensional $\boldsymbol{t}$-distributions. The important and difficult part of this calculation is the determination of the posterior distributions in the presence of incomplete observations due to the possibly unequal allocation of the budget.

Alloc: The expressions forming the Bonferroni lower bound for the PCS may be used to identify pairs of solutions for which the comparison has a large error probability and which need more data for a clear R&S decision. This results in a simple allocation rule that is simpler to calculate and turned out to be more efficient in our experiments than greedy OCBA allocation rules as they are often used in literature (see e.g. Branke et al. [2007]).

This paper is based on the doctoral thesis of one of the authors (Görder [2012]). It is organized along the three issues outlined above as follows. **Depend**: in the first Section we give the exact mathematical description of the sampling process and describe our Bayesian model. Details of the rather involved calculation of the posterior distribution with missing data are summarized in an Appendix. **Target**: the second Section generalizes the concept of ranking and selection of solutions to the case of partial selections. **Alloc**: in Section 3 we introduce several schemes for allocating the simulation budget to solutions based on the posterior distributions. A precise definition of our complete ranking and selection algorithm is given in Section 4. We report on extensive empirical tests with this algorithm in Section 5 where we compare it to a greedy type of OCBA algorithm and to the standard $\mathcal{KN}$++ procedure of Kim and Nelson [2006a]. Some conclusions are given in the final Section.

2 The Mathematical Model

2.1 A Bayesian Environment

Let $\mathcal{L} := \{1, \ldots, L\}$ denote the fixed set of solutions. X_{ik} is the k-th observation of solution $i \in \mathcal{L}$, i.e. the cost when i is applied to the k-th random scenario. We do not consider cost functions and scenarios explicitely in the sequel. We collect the X_{ik} into a matrix-like object $\boldsymbol{X}$: a column in our data $\boldsymbol{X}$ represents the observations of all solutions with a single scenario, whereas the rows represent all observations from a particular solution. $\boldsymbol{X}$ need not be a complete matrix: due to possibly unequal allocation of simulations we may have a ragged right

border, see below. As we use CRN, missing values at the end of a row are not really 'missing' but are rather 'not yet observed'.

Simulating *all* of the solutions from $\mathcal{L}$ with the k-th scenario therefore leads to a (column) vector of observations

$$\boldsymbol{X}_{\cdot\, k} := (X_{1k}, \ldots, X_{Lk})^T, \quad k = 1, 2 \ldots . \tag{2.1}$$

As it is often done in ranking and selection, we assume that $\boldsymbol{X}_{\cdot\, 1}, \boldsymbol{X}_{\cdot\, 2}, \ldots$ are independent and identically $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$-distributed observations. Here, $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ denotes the L-dimensional normal distribution with mean $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_L)^T \in \mathbb{R}^L$ and the positive definite $L \times L$ covariance matrix $\boldsymbol{\Sigma} := (\sigma_{ij})_{i,j=1,\ldots,L}$. This model includes the case, where the L solutions are simulated independently (i.e. with different scenarios), then $\boldsymbol{\Sigma}$ is a diagonal matrix. $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are assumed to be unknown.

Our overall goal is to extract information about $\boldsymbol{\mu}$ from the observations $\boldsymbol{X}$. Typically, we want to identify solutions $i \in \mathcal{L}$ that have small mean values μ_i.

We take a Bayesian point of view, that is we assume that the unknown parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are themselves observations of random variables W and S having a prior distribution with density $\pi(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. We do not assume any specific prior knowledge about the parameters, therefore we shall use the so-called uninformed prior distribution (see DeGroot [2004], Berger [1985]) with

$$\pi(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \;\propto\; \det(\boldsymbol{\Sigma})^{-\frac{\nu_0 + L + 1}{2}} \tag{2.2}$$

where $\propto$ means that the right hand side gives the density π up to some multiplicative constant that does not depend on $\boldsymbol{\mu}$ or $\boldsymbol{\Sigma}$. ν_0 is a so-called hyperparameter that allows to control the degree of uncertainty about $\boldsymbol{\Sigma}$.

2.2 Iterative allocation of simulation runs

Instead of simulating all solutions equally often, we iteratively allocate a given amount b of simulations to the solutions, depending on the observations seen so far, see the detailed algorithm in Section 5 below. The result are samples that may contain different numbers of observations for different solutions. We use

$$\boldsymbol{X}_{i\cdot} := (X_{i1}, X_{i2}, \ldots, X_{in_i}) \tag{2.3}$$

to denote the random (row) vector of the n_i observations produced for the i-th solution, $i = 1, \ldots, L$, and similarly $\boldsymbol{x}_{i\cdot} := (x_{i1}, x_{i2}, \ldots, x_{in_i})$ for a specific sample.

Let $\boldsymbol{n} = (n_1, \ldots, n_L) \in \mathbb{N}^L$ be the vector of the L present sample sizes, then the overall samples can be collected into a matrix-like scheme with possibly different row lengths n_i :

$$\boldsymbol{x}_{(\boldsymbol{n})} := \boldsymbol{x}_{(n_1,\ldots,n_L)} := \begin{pmatrix} x_{11}, & x_{12}, & \ldots & x_{1n_1} \\ x_{21}, & x_{22}, & \ldots & x_{2n_2} \\ \vdots & \vdots & & \vdots \\ x_{L1}, & x_{L2}, & \ldots & x_{Ln_L} \end{pmatrix}. \tag{2.4}$$

Columns $\boldsymbol{x}_{\cdot k}$ may be incomplete, as the k-th simulation (scenario) may not have been allocated to all solutions, see Figure 2.1 for an illustration. Let $\mathbb{R}^{L\otimes\boldsymbol{n}}$ denote the set of possible samples of that shape for a particular size vector $\boldsymbol{n} = (n_1, \ldots, n_L)$.

We shall now define the possible samples and allocation rules recursively. At first (in iteration 0), all solutions are simulated n_0 times where n_0 is a given fixed number. With $\boldsymbol{n}^{(0)} := (n_0, \ldots, n_0)$ we are therefore observing a ($(L \times n_0)$-matrix) sample $\boldsymbol{x}_{(\boldsymbol{n}^{(0)})} = \boldsymbol{x}_{(n_0,\ldots,n_0)}$ from

$$\mathcal{Z}_0 := \mathbb{R}^{L\otimes\boldsymbol{n}^{(0)}}.$$

Next we apply an *allocation rule* M_1

$$M_1 : \mathcal{Z}_0 \to \mathbb{N}^L \quad \text{with} \quad M_1(\boldsymbol{x}_{(\boldsymbol{n}^{(0)})}) =: (m_1^{(1)}, \ldots, m_L^{(1)})$$

that determines the numbers $m_i^{(1)}$ of additional simulations for solution $i = 1, \ldots, L$ in the first iteration. Then the overall number of simulations seen so far is

$$\boldsymbol{n}^{(1)} = (n_1^{(1)}, \ldots, n_L^{(1)}) := (n_0 + m_1^{(1)}, \ldots, n_0 + m_L^{(1)}).$$

After these additional simulations have been performed we have a sample

$$\boldsymbol{x}_{(\boldsymbol{n}^{(1)})} = \begin{pmatrix} x_{11} & x_{12} & \ldots & x_{1n_1^{(1)}} \\ x_{21} & x_{22} & \ldots & x_{2n_2^{(1)}} \\ \vdots & \vdots & & \vdots \\ x_{L1} & x_{L2} & \ldots & x_{Ln_L^{(1)}} \end{pmatrix}.$$

Let $\mathcal{Z}_1$ be the set of all possible samples after the first iteration, i.e.

$$\mathcal{Z}_1 := \bigcup_{\boldsymbol{x}\in\mathcal{Z}_0} \Big(\{\boldsymbol{x}\} \oplus \mathbb{R}^{L\otimes M_1(\boldsymbol{x})} \Big),$$

where the operation $\oplus$ concatenates elements row-wise, i.e.

$$\begin{aligned} \{\boldsymbol{x}_{(\boldsymbol{n})}\} \oplus \{\boldsymbol{y}_{(\boldsymbol{m})}\} &= \begin{pmatrix} x_{11} & \ldots & x_{1n_1} \\ x_{21} & \ldots & x_{2n_2} \\ \vdots & & \vdots \\ x_{L1} & \ldots & x_{Ln_L} \end{pmatrix} \oplus \begin{pmatrix} y_{11} & \ldots & y_{1m_1} \\ y_{21} & \ldots & y_{2m_2} \\ \vdots & \vdots & \\ y_{L1} & \ldots & y_{Lm_L} \end{pmatrix} \\ &= \begin{pmatrix} x_{11} & \ldots & x_{1n_1} & y_{11} & \ldots & y_{1m_1} \\ x_{21} & \ldots & x_{2n_1} & y_{21} & \ldots & y_{2m_2} \\ \vdots & & \vdots & \vdots & & \vdots \\ x_{L1} & \ldots & x_{Ln_L} & y_{L1} & \ldots & y_{Lm_L} \end{pmatrix}. \end{aligned}$$

Generally, after the t-th iteration we have a sample $\boldsymbol{x}_{(\boldsymbol{n}^{(t)})}$ where $\boldsymbol{n}^{(t)} = (n_1^{(t)}, \ldots, n_L^{(t)})$ gives the total number of simulations performed with each solution so far. Then,

an allocation rule $M_{t+1} : \mathcal{Z}_t \to \mathbb{N}^L$ is applied to determine the numbers of additional simulations in the $(t+1)$-st iteration. The set of possible samples after that iteration is

$$\mathcal{Z}_{t+1} := \bigcup_{\boldsymbol{x} \in \mathcal{Z}_t} \left(\{\boldsymbol{x}\} \oplus \mathbb{R}^{L \otimes M_{t+1}(\boldsymbol{x})} \right) .$$

Note, that under CRN the simulation of different iterations will in general not be independent as we may have to *reuse* scenarios (random numbers) for some solutions that have already been used in earlier iterations for other solutions. A new independent scenario is drawn for the simulation of some solution i only if i has been applied to all scenarios drawn before. See Figure 2.1 for a simple example.

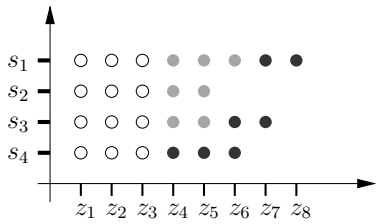

Figure 2.1: The first three iterations of a sampling scheme with $L = 4, n_0 = 3$ and budget $b = 7$. The allocations of the second iteration are marked in gray, those of the third in black. The results in the (complete) columns $1, \ldots, 5$ are i.i.d. $\mathbb{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$-distributed.

The allocation schemes we use below depend on the posterior distribution of the mean W given data $\boldsymbol{x} \in \mathcal{Z}_t$ which is determined in the next Subsection.

2.3 Likelihood with missing data

The likelihood function of incomplete samples as described in the last section are examined in great detail and generality in Dominici et al. [2000]. Our case is comparatively simple, as we have consecutive observations for each solution (row in the sample) and there are no 'holes', data may only be missing at the end of the sample. This is due to the CRN scheme we are using: assume a solution $i \in \mathcal{L}$ has been simulated with the first k scenarios resulting in $x_{i1}, \ldots, x_{ik}$. If no simulations are allocated to i in the next iterations, but additional simulations are performed in later iterations, these have to use scenarios $k+1, k+2, \ldots$ resulting in observations $x_{i,k+1}, x_{i,k+2}, \ldots$. Also, the pattern of the missing data is a function only of sample values observed before, this is called a monotone and ignorable pattern (Dominici et al. [2000]).

There is no closed expression for the posterior density of W given data $\boldsymbol{x} \in \mathcal{Z}_t$ if the covariance matrix $\boldsymbol{\Sigma}$ of the underlying Normal distribution is unknown. We therefore use a semi-Bayesian approach and first assume that the covariance matrix is known. We determine the conditional distribution of W given $\boldsymbol{X} = \boldsymbol{x}$ and $S = \boldsymbol{\Sigma}$ exactly and then replace $\boldsymbol{\Sigma}$ by its (non-Bayesian) estimate $\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})$.

To simplify notation, let the set of solutions $\mathcal{L} = \{1, \ldots, L\}$ be ordered such that for the present data $\boldsymbol{x} = \boldsymbol{x}_{(\boldsymbol{n})} \in \mathcal{Z}_t$ with $\boldsymbol{n} = (n_1, \ldots, n_L)$ we have

$$n_1 \geq n_2 \geq \cdots \geq n_L. \tag{2.5}$$

This means that solution 1 has been simulated with n_1 different independent scenarios. As we use CRN, the other solutions $i \in \{2, \ldots, L\}$ have been observed with subsets of these scenarios, see Fig. 2.2 for a simple example.

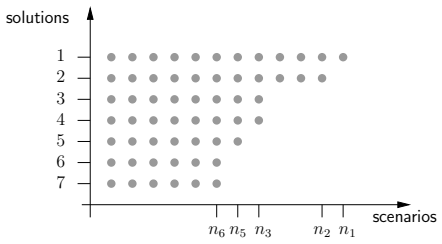

Figure 2.2: A sample with $\mathcal{L} = \{1, \ldots, 7\}$ and $n_1 = 12, n_2 = 11, n_3 = n_4 = 8, n_5 = 7, n_6 = n_7 = 6$.

We need projections of vectors and matrices to components corresponding to subsets of the solutions $\mathcal{L} = \{1, \ldots, L\}$. For $\boldsymbol{y} = (y_1, \ldots, y_L)^T \in \mathbb{R}^L$ and $i \in \{1, \ldots, L\}$ let

$$\boldsymbol{y}_{[<i]} := (y_1, \ldots, y_{i-1})^T \in \mathbb{R}^{i-1}, \quad \text{and} \quad \boldsymbol{y}_{[\leq i]} := (y_1, \ldots, y_i)^T \in \mathbb{R}^i. \tag{2.6}$$

Similarly, for the $L \times L$ matrix $\boldsymbol{\Sigma} = (\sigma_{k,l})_{k,l=1,\ldots,L}$ we define

$$\boldsymbol{\Sigma}_{[<i]} := (\sigma_{kl})_{k,l=1,\ldots,i-1}, \qquad \boldsymbol{\Sigma}_{[i,<i]} := (\sigma_{i1}, \ldots, \sigma_{i,i-1}) \quad \text{and} \tag{2.7}$$

$$\beta_i := \Sigma_{[i,<i]} \big(\Sigma_{[<i]}\big)^{-1}. \tag{2.8}$$

Here, β_i is a $(i-1)$-dimensional row vector. Let

$$\overline{\boldsymbol{x}}_i := \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij} \tag{2.9}$$

be the sample mean of all n_i observations $x_{i,1}, \ldots, x_{i,n_i}$ available for solution $i \in \{1, \ldots, L\}$. For $i < k$ we have $n_k \leq n_i$, therefore we may define the sample mean of solution i restricted to its first n_k observations

$$\overline{\boldsymbol{x}}_i^{(n_k)} := \frac{1}{n_k} \sum_{j=1}^{n_k} x_{ij}, \quad i = 1, \ldots, k-1. \tag{2.10}$$

Then $\overline{\boldsymbol{x}}_{[<i]}^{(n_i)} := (\overline{\boldsymbol{x}}_1^{(n_i)}, \ldots, \overline{\boldsymbol{x}}_{i-1}^{(n_i)})^T$ is the $(i-1)$-dimensional column vector of sample means restricted to the first n_i observations for solutions $1, \ldots, i-1$, that all have at least n_i observations, see Fig. 2.3.

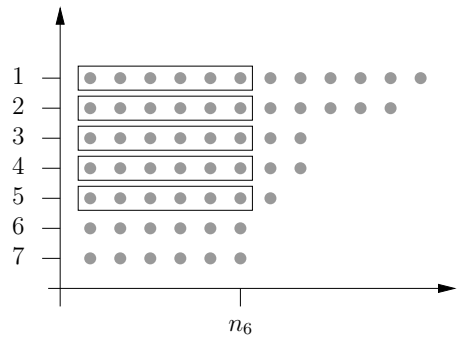

Figure 2.3: $\overline{\boldsymbol{x}}^{(n_6)}_{[<6]}$ contains all 5 sample means from the boxed values.

The posterior distribution of W given an incomplete observation $\boldsymbol{x}$ with known prior covariance is given in the following Theorem, its rather technical proof is sketched in the Appendix.

Theorem 1. Let (the columns) $\boldsymbol{X}_{\cdot k}, k = 1, 2, \ldots$ be i.i.d. $\mathbb{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distributed with *known* covariance matrix $\boldsymbol{\Sigma}$ and unknown mean $\boldsymbol{\mu}$. Assume that the variable W for the mean has the uninformative prior $\pi(\mu) \propto 1$. Let the (possibly incomplete) data $\boldsymbol{x} = \boldsymbol{x}_{(\boldsymbol{n})} \in \mathcal{Z}_t$ with $\boldsymbol{n} = (n_1, \ldots, n_L)$, $n_1 \geq n_2 \geq \cdots \geq n_L$ for some $t \in \mathbb{N}$, be given as described in Section 2.2.

Then the posterior distribution of W given $\boldsymbol{X} = \boldsymbol{x}$ is an L-dimensional Normal distribution $\mathcal{N}_L(\boldsymbol{\nu}, \boldsymbol{\Lambda})$ with mean $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_L)$ where

$$\nu_1 := \bar{\boldsymbol{x}}_1, \qquad \nu_i := \bar{\boldsymbol{x}}_i + \beta_i(\boldsymbol{\nu}_{[<i]} - \bar{\boldsymbol{x}}^{(n_i)}_{[<i]}) \quad \text{for } i = 2, \ldots, L, \tag{2.11}$$

and covariance matrix $\boldsymbol{\Lambda} := \boldsymbol{\Lambda}_{[\leq L]}$ where

$$\boldsymbol{\Lambda}_{[\leq 1]} = \frac{\sigma_{11}}{n_1}, \qquad \boldsymbol{\Lambda}_{[\leq i]} = \left(\begin{array}{c|c} \boldsymbol{\Lambda}_{[<i]} & \boldsymbol{\Lambda}_{[<i]}\ \beta_i^T \\ \hline \beta_i\ \boldsymbol{\Lambda}_{[<i]} & \frac{1}{n_i}(\sigma_{ii} - \beta_i \boldsymbol{\Sigma}_{[<i]} \beta_i^T) + \beta_i\ \boldsymbol{\Lambda}_{[<i]}\ \beta_i^T \end{array} \right) \tag{2.12}$$

for $i = 2, \ldots, L$.

For the case of an *unknown* covariance matrix $\boldsymbol{\Sigma}$ we have to replace $\boldsymbol{\Sigma}_{[<i]}$ and β_i by their estimators $\hat{\boldsymbol{\Sigma}}_{[<i]}(\boldsymbol{x})$ and $\hat{\beta}_i(\boldsymbol{x})$. For the estimation of $\boldsymbol{\Sigma}_{[<i]} = \big(\sigma_{kl}\big)_{1 \leq k,l < i}$ we only consider solutions $1, \ldots, i-1$. These all have sample sizes $\geq n_{i-1}$, we may therefore define for $1 \leq k, l \leq j \leq L$ and $\boldsymbol{x} = \boldsymbol{x}_{(\boldsymbol{n})}$ the estimator

$$\hat{\sigma}^{(n_j)}_{kl} = \hat{\sigma}^{(n_j)}_{kl}(\boldsymbol{x}) := \frac{1}{n_j} \sum_{m=1}^{n_j} (x_{km} - \bar{\boldsymbol{x}}^{(n_j)}_k)(x_{lm} - \bar{\boldsymbol{x}}^{(n_j)}_l) \tag{2.13}$$

and put

$$\begin{aligned} \hat{\boldsymbol{\Sigma}}_{[<i]} = \hat{\boldsymbol{\Sigma}}_{[<i]}(\boldsymbol{x}) &:= \left(\hat{\sigma}^{(n_{i-1})}_{kl}\right)_{k,l=1,\ldots,i-1} \\ \hat{\boldsymbol{\Sigma}}_{[i,<i]} = \hat{\boldsymbol{\Sigma}}_{[i,<i]}(\boldsymbol{x}) &:= (\hat{\sigma}^{(n_{i-1})}_{i1}, \ldots, \hat{\sigma}^{(n_{i-1})}_{i,i-1}). \end{aligned} \tag{2.14}$$

Note that we use the Maximum-Likelihood estimator for the covariances and that $\hat{\boldsymbol{\Sigma}}_{[<i]}$ is not necessarily contained in $\hat{\boldsymbol{\Sigma}}_{[<i+1]}$ as both estimators may use different sample sizes n_{i-1} and n_i. We also have to estimate the β_i and put

$$\hat{\beta}_i = \hat{\beta}_i(\boldsymbol{x}) := \hat{\boldsymbol{\Sigma}}_{[i,<i]}(\hat{\boldsymbol{\Sigma}}_{[<i]})^{-1}, \tag{2.15}$$

where we have to make sure that $\hat{\boldsymbol{\Sigma}}_{[<i]}$ is non singular. From Dykstra [1970] it is known, that if the sample size n_{i-1} of $\hat{\boldsymbol{\Sigma}}_{[<i]}$ fulfills $n_{i-1} > i-1$ then $\hat{\boldsymbol{\Sigma}}_{[<i]}$ is positive definite with probability one. This could be guaranteed if we require that the initial sample size n_0 is larger than the number of solutions L as then $n_{i-1} \geq n_0 > L \geq i-1$.

We may now plug these estimators into the definition of the posterior means and obtain

$$\hat{\nu}_1 = \hat{\nu}_1(\boldsymbol{x}) := \bar{\boldsymbol{x}}_1, \quad \hat{\nu}_i = \hat{\nu}_i(\boldsymbol{x}) := \bar{\boldsymbol{x}}_i + \hat{\beta}_i(\hat{\boldsymbol{\nu}}_{[<i]} - \bar{\boldsymbol{x}}^{(n_i)}_{[<i]}), \quad \hat{\boldsymbol{\nu}}(\boldsymbol{x}) := (\hat{\nu}_1, \ldots, \hat{\nu}_L). \tag{2.16}$$

To obtain an adequate estimator $\hat{\boldsymbol{\Lambda}}$ we first look at the case of *complete* observations, i.e. with $n_1 = \cdots = n_L > L$. Then it is well-known (see e.g. DeGroot [2004], 10.3) that with $\boldsymbol{\Sigma}$ *known* and an uninformative prior distribution for the mean W, the posterior distribution of W would be Normal with covariance matrix $\frac{1}{n_L}\boldsymbol{\Sigma}$. If $\boldsymbol{\Sigma}$ is *unknown* with the improper prior distribution as in (2.2) the marginal posterior distribution of the mean W in the complete observation case is an L-dimensional $\boldsymbol{t}$-distribution with $n_L - L + \nu_0$ degrees of freedom, location parameter $\bar{\boldsymbol{x}}$ and scale matrix $\frac{1}{n_L - L + \nu_0}\hat{\boldsymbol{\Sigma}}(\boldsymbol{x})$. Here, the correction term $\frac{1}{n_L - L + \nu_0}$ involves the hyperparameter ν_0, the sample size and the dimension of the problem. For the present situation of incomplete observations and *known* covariance matrix, the posterior covariance $\frac{1}{n_L}\boldsymbol{\Sigma}$ has to be replaced by $\boldsymbol{\Lambda}$ as in (2.12), reflecting the different sample sizes for each solution instead of the fixed size n_L. Then, in the case of *unknown* $\boldsymbol{\Sigma}$, it seems reasonable to approximate the posterior distribution of the mean W by an L-dimensional $\boldsymbol{t}$-distribution with $n_L - L + \nu_0$ degrees of freedom and location parameter $\hat{\boldsymbol{\nu}}(\boldsymbol{x})$. The scale matrix should be obtained from $\boldsymbol{\Lambda}$ with the σ_{kl} replaced by their adequate estimators. In particular, the correction terms $\frac{1}{n_L - L + \nu_0}$ from the complete observation case should be replaced on the i-th step of the recursion in (2.12) by $\frac{1}{n_i - i + \nu_0}$ using the number i of solutions considered in that step. We thus obtain

$$\hat{\boldsymbol{\Lambda}}_{[\leq 1]} = \hat{\boldsymbol{\Lambda}}_{[\leq 1]}(\boldsymbol{x}) := \frac{\hat{\sigma}^{(n_1)}_{11}}{n_1 - 1 + \nu_0}, \tag{2.17}$$

$$\hat{\boldsymbol{\Lambda}}_{[\leq i]} = \hat{\boldsymbol{\Lambda}}_{[\leq i]}(\boldsymbol{x}) := \left(\begin{array}{c|c} \hat{\boldsymbol{\Lambda}}_{[<i]} & \hat{\boldsymbol{\Lambda}}_{[<i]}\ \hat{\beta}_i^T \\ \hline \hat{\beta}_i\ \hat{\boldsymbol{\Lambda}}_{[<i]} & \frac{1}{n_i - i + \nu_0}(\hat{\sigma}^{(n_i)}_{ii} - \hat{\beta}_i \hat{\boldsymbol{\Sigma}}_{[<i]} \hat{\beta}_i^T) + \hat{\beta}_i\ \hat{\boldsymbol{\Lambda}}_{[<i]}\ \hat{\beta}_i^T \end{array}\right)$$

for $i = 2, \ldots, L$, and $\hat{\boldsymbol{\Lambda}} = \hat{\boldsymbol{\Lambda}}(\boldsymbol{x}) := \hat{\boldsymbol{\Lambda}}_{[\leq L]}(\boldsymbol{x})$.

In this paper, the posterior distribution of the mean W is used mainly to express the probability of a wrong selection, see below. In particular, we need

the posterior probability of the event $W_i \leq W_j + \delta$ for $1 \leq i, j \leq L$ and $\delta \geq 0$. From the properties of the multivariate $\boldsymbol{t}$-distribution we may conclude that

$$\begin{aligned} \mathbf{P}[W_i \leq W_j + \delta \mid \boldsymbol{X} = \boldsymbol{x}] \;&=\; \mathbf{P}[W_i - W_j \leq \delta \mid \boldsymbol{X} = \boldsymbol{x}] \\ &\approx\; G(\delta;\; \min\{n_i, n_j\} - 1,\; \hat{\nu}_i - \hat{\nu}_j,\; \hat{\Lambda}_{ii} + \hat{\Lambda}_{jj} - 2\hat{\Lambda}_{ij}) \\ &:= p_{ij}^{\delta} \end{aligned} \tag{2.18}$$

where $G(\cdot\;; k, a, b)$ is the distribution function of the one-dimensional t-distribution with k degrees of freedom, location parameter a and scale parameter b. This approximation will be used below.

3 General Ranking and Selection Schemes

3.1 Target and Selection

We start with a general definition of the ranking and selection schemes we are examining in this paper. It is a generalization of the approach in Schmidt et al. [2006].

We want to select solutions from the set $\mathcal{L} = \{1, \ldots, L\}$ according to their ranks under some performance measure, in our case the mean value. E.g. we want to select the solution with the lowest mean value (the best solution) or the m best solutions as it is often used e.g. in ant algorithms. We restrict ourselves to such selections that can be determined using pairwise comparisons of solutions only. The idea is to formulate *minimal* requirements for the correctness of a selection in terms of pairwise comparisons and then use (2.18) to determine the error probability. This may allow a tighter error bound compared to a complete ranking of all solutions. We first introduce an abstract concept which is illustrated by an example below.

For a general ranking and selection scheme (R&S-scheme) we first define a set of *target ranks* $A \subset \{1, \ldots, L\}$. This means that we want to select those solutions that have ranks from A with respect to their mean values. As the mean values are assumed to be unknown, we use their available estimates $\hat{\nu}_1(\boldsymbol{x}), \ldots, \hat{\nu}_L(\boldsymbol{x})$ instead. These are ordered in increasing order

$$\hat{\nu}_{i_1}(\boldsymbol{x}) \leq \hat{\nu}_{i_2}(\boldsymbol{x}) \leq \cdots \leq \hat{\nu}_{i_L}(\boldsymbol{x}) \tag{3.1}$$

and the solutions with estimated ranks in A are selected, i.e. the solutions

$$B = B(\boldsymbol{x}) := \{i_j \mid j \in A\}. \tag{3.2}$$

The aim is then to determine the error probability of the selection B, i.e. the posterior probability that a solution $l \in B$ does not have a rank from A.

As we have continuous posterior distributions for which

$$\mathbf{P}[W_i = W_j \text{ for some } i \neq j \mid \boldsymbol{X} = \boldsymbol{x}] = 0 \tag{3.3}$$

we may restrict ourselves to the L-dimensional Euclidean space without equal values:

$$\mathbb{R}^{L*} := \{\boldsymbol{t} = (t_1, \ldots, t_L) \in \mathbb{R}^L \mid t_i \neq t_j \text{ for all } i \neq j\}. \tag{3.4}$$

Let

$$C_{AB} := \Big\{\boldsymbol{t} \in \mathbb{R}^{L*} \mid \{\text{rank}(t_l) \mid l \in B\} = A\Big\} \tag{3.5}$$

be the set of all L-dimensional vectors, in which the selected positions from B have ranks A. Thus, C_{AB} is the set of all potential means for which the selection B would be correct for target A. Recall that $W = (W_1, \ldots, W_L)$ is the random variable indicating the unknown mean. With the help of C_{AB} we can therefore express the probability that B is a correct selection for target A simply as

$$\mathbf{P}[W \in C_{AB} \mid \boldsymbol{X} = \boldsymbol{x}] = \mathbf{P}[\{\text{rank}(W_l) \mid l \in B\} = A \mid \boldsymbol{X} = \boldsymbol{x}].$$

For an easier access to this probability we assume that there is a binary *relation*

$$\rho_{AB} \quad \subset \quad [B \times (\mathcal{L} - B)] \ \cup \ [(\mathcal{L} - B) \times B] \tag{3.6}$$

on pairs (l, j) that relates selected positions $l \in B$ to unselected positions $j \in \mathcal{L} - B$, such that C_{AB} has the following representation

$$C_{AB} = \big\{t \in \mathbb{R}^{L*} \mid \forall\ (i,j) \in \mathcal{L}^2 \quad \big(\rho_{AB}(i,j) \Rightarrow t_i \leq t_j\big)\big\} \tag{3.7}$$

where as usual $\rho_{AB}(i,j)$ is true if $(i,j) \in \rho_{AB}$. Thus ρ_{AB} provides a definition of a correct selection by pairwise comparison of certain pairs (W_i, W_j). Note that B and hence C_{AB} and ρ_{AB} all depend on the observation $\boldsymbol{x}$. The following examples explain these definitions.

Example 1. Assume that (3.1) holds.

a) Let $A := A_{\text{best}} := \{1\}$, this means we want to select the best solution. Then with (3.1), the selection is $B := \{i_1\}$ as $\hat{\nu}_{i_1}(\boldsymbol{x})$ is the smallest posterior mean. With

$$\rho_{AB} := \{(i_1, j) \mid j \in \mathcal{L} - \{i_1\}\}$$

we have from (3.7)

$$C_{AB} := \{\boldsymbol{t} \in \mathbb{R}^{L*} \mid t_{i_1} \leq t_j \text{ for all } j \neq i_1\}.$$

C_{AB} is the set of all potential mean value vectors where selection $B = \{i_1\}$ leads to the best (minimal) solution.

b) If $A := A_{\text{m-best}} := \{1, \ldots, m\}$ for some $m \leq L$ we want to select the m best (minimal) solutions. Then from (3.1) we see that we must choose $B := \{i_1, \ldots, i_m\}$. As characterizing relation we obtain

$$\rho_{AB} := B \times (\mathcal{L} - B) = \{(l, j) \mid l \in B, j \in \mathcal{L} - B\}$$

and

$$C_{AB} := \{\boldsymbol{t} \in \mathbb{R}^{L*} \mid t_l \leq t_j \text{ for all } l \in B, j \notin B\}.$$

c) If, in addition, the m best solutions have to be ranked among themselves then we would choose

$$\rho_{AB} := \{(i_1, i_2), (i_2, i_3) \ldots, (i_{m-1}, i_m)\} \cup \{(i_m, j) \mid j \notin B\}$$

and

$$C_{AB} := \{\boldsymbol{t} \in \mathbb{R}^{L*} \mid t_{i_1} \leq t_{i_2} \leq \cdots \leq t_{i_m} \text{ and } t_{i_m} \leq t_l, l \in \mathcal{L} - B\}.$$

This example includes complete ranking of the solution with $m := L$ and

$$\rho_{AB} := \{(i_1, i_2), (i_2, i_3) \ldots, (i_{L-1}, i_L)\}.$$

d) If we want to select the median with $A := A_{\text{median}} = \{\lceil L/2 \rceil\}$, we take as selection $B := \{i_{\lceil L/2 \rceil}\} =: \{l_0\}$, the median solution with respect to posterior means (3.1) and as auxiliary sets $B_1 := \{i_1, \ldots, i_{\lceil L/2 \rceil - 1}\}$ and $B_2 := \{i_{\lceil L/2 \rceil + 1}, \ldots, i_L\}$. Then we use as characterizing relation

$$\rho_{AB} := \{(j, l_0) \mid j \in B_1\} \ \cup \ \{(l_0, j) \mid j \in B_2\}$$

and obtain

$$C_{AB} = \{\boldsymbol{t} \in \mathbb{R}^{L*} \mid t_j \leq t_{l_0} \text{ for } j \in B_1 \text{ and } t_{l_0} \leq t_j \text{ for } j \in B_2\}$$

as the set of vectors from $\mathbb{R}^{L*}$ where about half of the components is less than t_{l_0} and the rest is larger, therefore t_{l_0} is the median.

e) As a final example let $A := A_{span} := \{1, L\}$ denote a target that could be used to describe the span of the mean values of the solution. Then the selection should be $B = \{i_1, i_L\}$ from (3.1) and

$$\rho_{AB} := \{(i_1, j) \mid j \in \mathcal{L} - B\} \ \cup \ \{(j, i_L) \mid j \in \mathcal{L} - B\}$$

and

$$C_{AB} := \{\boldsymbol{t} \in \mathbb{R}^{L*} \mid t_{i_1} \leq t_j \leq t_{i_L} \text{ for all } j \neq i_1, i_L\}.$$

In the iterative procedure below, the posterior means $\hat{\nu}_1(\boldsymbol{x}), \ldots, \hat{\nu}_L(\boldsymbol{x})$ have to be determined after each iteration based on the new observations. Therefore, B, ρ_{AB} and C_{AB} have to be adapted in each iteration also.

3.2 The Probability of a Correct Selection

We now define the probability of correct selection (PCS) for a selection as in (3.2) simply by

$$PCS := \mathbf{P}[W \in C_{AB} \mid \boldsymbol{X} = \boldsymbol{x}]. \tag{3.8}$$

To determine PCS directly, one has to solve high dimensional integrals in order to arrive at the marginal distribution of the posterior distribution on the components of the selection B. Instead, we use the relation ρ_{AB} that defines the set

C_{AB} to derive a simple lower bound of Bonferroni type for the PCS as follows

$$\begin{aligned} PCS &= \mathbf{P}[W \in C_{AB} \mid \boldsymbol{X} = \boldsymbol{x}] \\ &= \mathbf{P}\Big[W_i \le W_j \text{ for all } 1 \le i,j \le L \text{ with } \rho_{AB}(i,j) \mid \boldsymbol{X} = \boldsymbol{x}\Big] \\ &= 1 - \mathbf{P}\Big[W_i > W_j \text{ for some } 1 \le i,j \le L \text{ with } \rho_{AB}(i,j) \mid \boldsymbol{X} = \boldsymbol{x}\Big] \\ &\ge 1 - \sum_{(i,j)\in\rho_{AB}} \mathbf{P}[W_i > W_j \mid \boldsymbol{X} = \boldsymbol{x}] \qquad (3.9) \\ &= 1 - \sum_{(i,j)\in\rho_{AB}} \big(1 - \mathbf{P}[W_i - W_j \le 0 \mid \boldsymbol{X} = \boldsymbol{x}]\big). \end{aligned}$$

Using (2.18) we may approximate this lower bound by the following expression

$$LB(\boldsymbol{x}) := 1 - \sum_{(i,j)\in\rho_{AB}} (1 - p_{ij}^0) \qquad (3.10)$$

It is quite usual in ranking and selection to relax the definition of correctness of a selection. Instead of strict comparisons of means $W_i < W_j$ for relevant pairs $(i,j) \in \rho_{AB}$ we are content if $W_i < W_j + \delta$ for some fixed *indifference zone* value $\delta > 0$. This allows to take the limited precision of our observations into account. Formally, we then define

$$C_{AB}^{\delta} := \Big\{ \boldsymbol{t} \in \mathbb{R}^{L*} \mid t_i < t_j + \delta \text{ for all } (i,j) \text{ with } \rho_{AB}(i,j) \Big\}$$

and have, using (2.18)

$$\begin{aligned} PCS^{\delta} &:= \mathbf{P}[W \in C_{AB}^{\delta} \mid \boldsymbol{X} = \boldsymbol{x}] \\ &\ge 1 - \sum_{(i,j)\in\rho_{AB}} \mathbf{P}[W_i > W_j + \delta \mid \boldsymbol{X} = \boldsymbol{x}] \\ &\approx 1 - \sum_{(i,j)\in\rho_{AB}} \big(1 - G(\delta; \min\{n_i, n_j\} - 1,\ \hat{\nu}_i - \hat{\nu}_j,\ \hat{\Lambda}_{ii} + \hat{\Lambda}_{jj} - 2\hat{\Lambda}_{ij})\big) \qquad (3.11) \\ &= 1 - \sum_{(i,j)\in\rho_{AB}} (1 - p_{ij}^{\delta}) \ =: LB^{\delta}(\boldsymbol{x}) \end{aligned}$$

4 Allocation strategies

In each of the iterations described in Section 2.2 it has to be decided how many simulations q_i should be performed for each solution $i \in \mathcal{L}$. We first look at a modified version of the so-called optimal computing budget allocation (OCBA) strategy introduced by Chen (see for example Chen and Lee [2010], Chen et al. [2000, 2008]). OCBA allocation strategies try to allocate a fixed simulation budget $b \in \mathbb{N}$ in such a way that the expected value of the PCS is maximized.

Let $\boldsymbol{q} = (q_1, \ldots, q_L) \in \mathbb{N}^L$ with $\sum_{i=1}^{L} q_i = b$ denote an allocation of the b simulations to solutions $\mathcal{L} = \{1, \ldots, L\}$. Calculating the expected effect of

additional simulations and to find q_i that are strictly optimal with respect to that expectation is a difficult non-linear optimization problem, see e.g. Chen and Yucesan [2005]. Therefore, most versions of the OCBA in the literature solve a substitute problem and try to maximize an approximation $\tilde{LB}(\boldsymbol{x};\boldsymbol{q})$ to the lower bound as in (3.9) for given data $\boldsymbol{x}$ and additional simulations $\boldsymbol{q}$. In this sense, a myopically optimal allocation is the solution to the following optimization problem:

$$\begin{aligned} &\text{maximize} && \tilde{LB}(\boldsymbol{x};\boldsymbol{q}) \\ &\text{subject to} && \sum_{i=1}^{L} q_i = b, \quad q_i \in \mathbb{N}. \end{aligned} \tag{4.1}$$

In general, even this simplified problem can be solved exactly only for very small instances of $\mathcal{L}$ and small simulation budgets b. For larger instances, heuristic solution approaches must be used, see e.g. [Branke et al., 2007, Chen et al., 1996, 1997].

We adapt this approach to our environment with dependent observations. The difficulty lies in estimating the future covariances *after* the additional simulations $\boldsymbol{q}$ have been performed. We use the lower bound

$$\tilde{LB}^{\delta}(\boldsymbol{x};\boldsymbol{q}) := 1 - \sum_{(i,j)\in\rho_{AB}} \left(1 - p_{ij}^{\delta}(q_i,q_j)\right) \quad \text{with} \tag{4.2}$$

$$p_{ij}^{\delta}(q_i,q_j) := G\left(\delta;\, \min\{n_i+q_i, n_j+q_j\} - 1\,, \hat{\nu}_j - \hat{\nu}_i,\, \Gamma_{ij}\right) \tag{4.3}$$

where the scale parameter Γ_{ij} is a weighted mean of the posterior covariances:

$$\begin{aligned} \Gamma_{ij} :=& \frac{n_i}{n_i+q_i}\hat{\Lambda}_{ii} + \frac{n_j}{n_j+q_j}\hat{\Lambda}_{jj} \\ & - 2\left[\frac{\hat{\Lambda}_{ii}}{\hat{\Lambda}_{ii}+\hat{\Lambda}_{jj}}\frac{n_i}{n_i+q_i} + \frac{\hat{\Lambda}_{jj}}{\hat{\Lambda}_{ii}+\hat{\Lambda}_{jj}}\frac{n_j}{n_j+q_j}\right]\hat{\Lambda}_{ij}. \end{aligned}$$

Here it is assumed that the posterior variance of $W_i - W_j$ after $\boldsymbol{q}$ additional simulations can be estimated from the present posterior values $\hat{\Lambda}_{ii}, \hat{\Lambda}_{jj}$ and $\hat{\Lambda}_{ij}$ by entering the variances $\hat{\Lambda}_{ii}, \hat{\Lambda}_{jj}$ inversely proportional to the relative increases of the sample sizes and by scaling the covariance $\hat{\Lambda}_{ij}$ such that the influence of the sample sizes n_i+q_i, n_j+q_j is proportional to the posterior variances $\hat{\Lambda}_{ii}$ and $\hat{\Lambda}_{jj}$.

A greedy heuristic (GreedyOCBA) to find good solutions to the problem (4.1) may then be defined similar as in Chen and Lee [2010] and Branke et al. [2007]. GreedyOCBA first measures the benefit of assigning all b additional simulations to a single solution $l \in \mathcal{L}$:

$$\begin{aligned} \Delta_l &:= \tilde{LB}^{\delta}(\boldsymbol{x};\, b\cdot\boldsymbol{e}_l) - \tilde{LB}^{\delta}(\boldsymbol{x},\boldsymbol{0}) \\ &= \sum_{j\in\mathcal{L}:(l,j)\in\rho_{AB}} \left[p_{lj}^{\delta}(b,0) - p_{lj}^{\delta}(0,0)\right] + \sum_{i\in\mathcal{L}:(i,l)\in\rho_{AB}} \left[p_{il}^{\delta}(0,b) - p_{il}^{\delta}(0,0)\right], \end{aligned}$$

where the $p^{\delta}_{i,j}(\cdot,\cdot)$ are defined in (4.2) and $\boldsymbol{e}_l$ is the l-th unit vector which has a 1 at the l-th position and zeros elsewhere. Then, GreedyOCBA distributes the simulation budget proportional to the weights Δ_l, i.e.

$$q_l := \left\lfloor b \cdot \frac{\Delta_l}{\sum_{i=1}^{L} \Delta_i} \right\rfloor, \quad l = 1, \ldots, L. \tag{4.4}$$

A remaining budget $R := b - \sum_{i=1}^{L} q_i$ is allocated according to the largest remainder method.

This allocation strategy requires $2 \cdot |\rho_{AB}|$ evaluations of the distribution function G in total. Hence its computational effort is about twice as high as the calculation of the Bonferroni bound LB in (3.10). This complexity can be reduced if we do not try to estimate the future PCS but simply look at its present value, more precisely its components $p^{\delta}_{ij} \approx \mathbf{P}[W_i \leq W_j + \delta \mid \boldsymbol{X} = \boldsymbol{x}]$, defined in (2.18). p^{δ}_{ij} describes the posterior probability of δ-dominance of W_i over W_j. Recall that for $(i,j) \in \rho_{AB}$ we have to make sure the δ-dominance $W_i \leq W_j + \delta$ in order for the present selection B to be correct with indifference parameter δ. Hence a small value of p^{δ}_{ij} for $(i,j) \in \rho_{AB}$ indicates that at least one of the solutions i, j has insufficient data. We therefore define the weights

$$\tilde{\Delta}_l := 1 - \min\left\{ p^{\delta}_{ij} \cdot \left(1 - \frac{\hat{\Lambda}_{ll}}{\hat{\Lambda}_{ii} + \hat{\Lambda}_{jj}}\right) \;\middle|\; (i,j) \in \rho_{AB},\ i = l \text{ or } l = j \right\}, \tag{4.5}$$

then the budget is allocated proportionally to these weights as above. Here, those solutions l get a larger weight that are part of a pair $(i,j) \in \rho_{AB}$ that has a small dominance probability and where the partner of l has a relatively small variance. This implies that l has a relatively large variance and hence needs more simulations to increase the certainty of the dominance relation (i,j). We call this strategy Dominance Probability Weighting ($\mathcal{DPW}$). In empirical tests $\mathcal{DPW}$ proved slightly better than GreedyOCBA with respect to the number of simulations needed, at the same time it needs less computational effort as only the p^{δ}_{ij} from the Bonferroni bound (3.11) are used.

It turned out in the experiments that the performance could be improved further by stopping simulations for those solutions with high enough dominance probabilities. Therefore we restricted the definition of $\tilde{\Delta}_l$ in (4.5) to those p^{δ}_{ij} which are below $1 - \alpha/|\rho_{AB}|$ where $|\rho_{AB}|$ is the number of summands in the Bonferroni bound (3.10). The allocation strategy $\mathcal{DPW}+$ therefore uses the weights

$$\tilde{\tilde{\Delta}}_l := 1 - \min\left\{ p^{\delta}_{ij} \cdot \left(1 - \frac{\hat{\Lambda}_{ll}}{\hat{\Lambda}_{ii} + \hat{\Lambda}_{jj}}\right) \;\middle|\; (i,j) \in \rho_{AB},\ i = l \text{ or } l = j,\ p^{\delta}_{ij} < 1 - \frac{\alpha}{|\rho_{AB}|} \right\}$$

and then allocates simulations as in (4.4). Empirical results on GreedyOCBA and $\mathcal{DPW}+$ are given in Section 6 below.

We are now in the position to define our algorithm in detail.

5 The Algorithm BayesRS

Let the following items be given:

$\mathcal{L} = \{1, \ldots, L\}$ is the set of solutions, $A \subset \{1, \ldots, L\}$ is the target set of ranks to be selected and possibly ranked, $\alpha \in (0, 1)$ is the bound for the error probability, $b \in \mathbb{N}$ is the simulation budget for each iteration, $n_0 \in \mathbb{N}$ is an initial sample size and δ is the indifference zone parameter.

Initialization : Observe $\boldsymbol{X}_{\cdot j}$ for $j = 1, \ldots, n_0$, i.e. choose n_0 random scenarios and apply all solutions to each of them. Let $\boldsymbol{x}$ denote the result.

Determine the posterior means $\hat{\nu}_j(\boldsymbol{x}), j \in \mathcal{L}$, as in (2.16), the selection $B(\boldsymbol{x})$ as in (3.2), relation ρ_{AB} as in (3.6) and (3.7) and the dominance probabilities $p^{\delta}_{ij}, (i, j) \in \rho_{AB}$, as in (2.18). Finally calculate the lower bound $LB^{\delta}(\boldsymbol{x})$ for the PCS as in (3.11).

while $LB^{\delta}(\boldsymbol{x}) < 1 - \alpha$ **do**

- apply an allocation rule M to determine the number of additional simulation runs $\boldsymbol{q} = (q_1, \ldots, q_L) := M(\boldsymbol{x})$,
- perform q_i simulations with solution $i \in \mathcal{L}$, taking into account the common random numbers scheme as described in Section 2.2, let $\boldsymbol{x}$ be the extended data including the new simulation results,
- update the posterior means $\hat{\boldsymbol{\nu}}(\boldsymbol{x})$, the selection $B(\boldsymbol{x})$, the relation ρ_{AB}, the dominance probabilities $p^{\delta}_{ij}, (i, j) \in \rho_{AB}$, and the lower bound $LB^{\delta}(\boldsymbol{x})$.

return the present selection $B(\boldsymbol{x})$.

In Görder [2012] it is shown that this algorithm terminates if at least one simulation is allocated to each solution in each iteration.

6 Computational study

We implemented the algorithm BayesRS and compared its efficiency to other R&S procedures. The main objectives of the study were:

- to compare different allocation strategies within the framework of BayesRS, here we use GreedyOCBA, $\mathcal{DPW}+$ and EqualAllocation, the naive equal allocation of the budget to solutions,
- to show the increasing efficiency of $\mathcal{DPW}+$ with increasingly positive correlation of the observations,
- to compare BayesRS with allocation rule $\mathcal{DPW}+$ to another standard from literature, namely $\mathcal{KN}++$, a procedure designed to find the best solution, see Kim and Nelson [2006b], and

- to investigate the behaviour of our approach in cases where there is no positive correlation. It seems that the (approximately) correct determination of the posterior distribution for missing values makes the allocation more precise, even if, in the case of negative correlation, common random numbers may increase the variance of the estimators used.

We measured the performance by the average number of simulations each strategy needs with a common error bound α. Also we checked the empirical error probabilities or rather PCS. The tests were implemented using the free statistics software `R`. In Görder [2012] further studies show the efficiency of these allocation strategies in the context of heuristic optimization methods like ant algorithms.

6.1 Test setup

As our methods require normally distributed observations, we generated them by a $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$-random generator for different values of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

Some values were fixed: the number of solutions $L = 20$ (other values showed similar behaviour), the error probability $\alpha = 0.05$ and the indifference zone parameter $\delta = 0.01$. The initial sample size was $n_0 := L+1 = 21$, the budget to be allocated in each iteration was $b = 10 \cdot L = 200$, and at least one simulation was allocated to each solution in each iteration. The parameter ν_0 for the prior probability of the covariance matrix as in (2.2) showed best results in our setup for $\nu_0 = L - 1 = 19$ and was therefore fixed to this value throughout our tests.

R&S-case	$\boldsymbol{\mu}$
Best_1	$\mu_1 = 0, \quad \mu_2 = \cdots = \mu_L = 1$
Best_{10}	$\mu_1 = \cdots = \mu_{10} = 0, \quad \mu_{11} = \cdots = \mu_L = 1$
Rank_{10}	$\mu_1 = 0, \mu_2 = 1, \ldots, \mu_{10} = 9, \mu_{11} = \cdots = \mu_L = 10$

Table 1: Different values for μ were used in the $\boldsymbol{\mu}$ -case "ufc".

A *basic scenario* consists of the following four variables that are varied in the tests:

1. We have examined three different **R&S-cases** : in "Best_1" we want to select the best solution, i.e. we use a target set $A = \{1\}$ (see subsection 3.1), in "Best_{10}" we want to select the better half of the solutions ($A = \{1, \ldots, 10\}$) and in "Rank_{10}" we also want to rank these ten best solutions.

2. Also three different **$\boldsymbol{\mu}$-cases** have been used for the $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$-generator. In the case "inc", $\boldsymbol{\mu}$ is the increasing sequence $\mu_1 = 0, \mu_2 = 1, \ldots, \mu_L = L-1$. In the unfavourable case "ufc", $\boldsymbol{\mu}$ is adapted to the R&S-case chosen as described in Table 1. In the case "unif", L values are drawn randomly from the interval $[0, 100]$ with a minimal distance of at least $\delta = 0.01$ and then sorted into increasing order. This is repeated $M_\mu := 15$ times,

so that 15 simulations with different random $\boldsymbol{\mu}$ are performed. As we use a Bayesian approach, the "unif"-case seems to be the most natural to simulate the uninformative prior but the cases may differ remarkably depending on how well the random values are separated.

3. As our method claims to work well when observations are positively correlated, we created covariance matrices $\boldsymbol{\Sigma} = \left(\sigma_{ij}\right)_{i,j=1,\ldots,L}$ for the $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$-generator with a given joint correlation $cor \in \{0.0, 0.2, 0.5, 0.7, 0.9\}$. To do so, variances $\sigma_{11}, \ldots, \sigma_{LL}$ were chosen uniformly distributed in the interval $[1, 10]$, then we put $\sigma_{ij} := cor\sqrt{\sigma_{ii}\sigma_{jj}}$ for $1 \leq i, j \leq L, i \neq j$. To examine the robustness of our procedure when there are negative correlations, we complemented the above construction for $cor \in \{-0.9, -0.5, -0.2\}$ with $\sigma_{ij} := (-1)^{i-j}|cor|\sqrt{\sigma_{ii}\sigma_{jj}}$ resulting in a covariance matrix with alternating positive and negative entries. Finally we used a random covariance matrix following a Wishart distribution with L degrees of freedom and a random scale matrix. These make nine different **$\boldsymbol{\Sigma}$-cases**.

4. Finally, we distinguish two **CRN-case**: we apply the complex calculation for the posterior means and covariances based on the joint distribution as described above (case "isCRN") or we simply use the marginal posterior distributions as if no CRN had been used. In this case ("noCRN") the posterior means and variances are estimated by standard non-Bayesian estimators. This would be correct in the uncorrelated case with $cor = 0.0$, but it is a simplification in the other cases.

This results in 162 different scenarios. For each scenario, $M_{cov} := 15$ random covariance matrices $\boldsymbol{\Sigma}$ were generated according to the $\boldsymbol{\Sigma}$-case chosen and, if the μ-case "unif" was used, also $M_\mu = 15$ random vectors $\boldsymbol{\mu}$ were generated. For each pair of $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, $M = 10$ repetitions of the different allocation strategies were performed. We kept track of the random seeds so that all strategies used the same random observations.

6.2 The unfavourable μ-case

We first show the results for $\boldsymbol{\mu}$-case "ufc" with CRN-case "isCRN". In Figure 6.1 the mean number of simulations necessary to obtain a PCS $\geq 1-\alpha$ with BayesRS is shown for the three allocation strategies EqualAllocation, GreedyOCBA and $\mathcal{DPW}+$. The x-axis shows the nine different cor-cases repeated for each of the three R&S-cases "Best_1", "Best_{10}" and "Rank_{10}". Here, the $\boldsymbol{\Sigma}$-case with the random covariance matrix is indicated by 'rnd'. The number of simulations on the y-axis is the mean over the $M_{cov} = 15$ different covariance matrices, each with the given correlation, and the $M = 10$ repetitions for each scenario.

Figure 6.1 clearly shows that the intelligent allocation rules are much more efficient than the simple equal allocation. Also in all scenarios, our new allocation rule $\mathcal{DPW}+$ performed better than the classical GreedyOCBA. This holds for all $\boldsymbol{\Sigma}$-cases, including the ones involving negative correlations as well

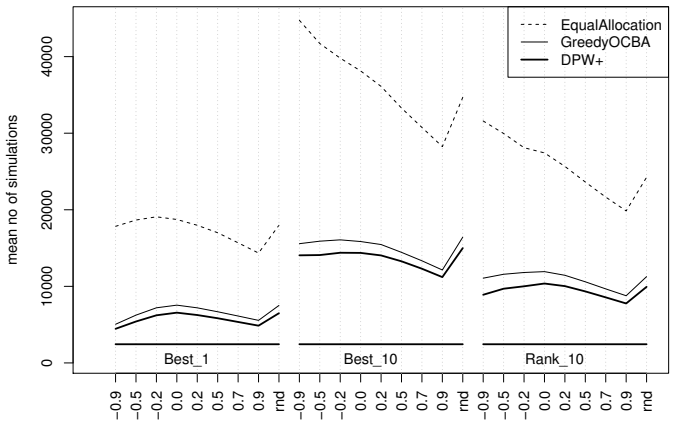

Figure 6.1: The unfavourable μ-case: comparison of the allocation strategies EqualAllocation, GreedyOCBA and $\mathcal{DPW}+$ using the full posterior distribution of the unknown means.

as the random covariance matrix. Increasing the correlation from 0.0 to 0.9 reduced the necessary effort, for all strategies.

Figure 6.2 shows $\boldsymbol{\mu}$-case "ufc" with CRN-case "noCRN". We use the same multi-normal observations as before, but this time the posterior distribution is based on the marginal distribution of the observation only, neglecting the possible dependence. In particular, the complicated definition of the posterior covariance matrix $\hat{\boldsymbol{\Lambda}}$ in (2.17) is replaced by a diagonal matrix $\tilde{\boldsymbol{\Lambda}}$ with diagonal $\hat{\sigma}_{ii}^{(n_i)}/(n_i - 1)$ as defined in (2.13). Note that this is justified only in the $\boldsymbol{\Sigma}$-case $cor = 0.0$, the only case where the observation for different solutions are independent. Nevertheless, Figure 6.2 shows a similar picture as Figure 6.1, $\mathcal{DPW}+$ is superior in all scenarios, but the absolute values of the number of simulations needed is larger.

In Figure 6.3 we therefore compare the CRN-cases "isCRN" and "noCRN" for the best allocation strategy $\mathcal{DPW}+$ and $\boldsymbol{\mu}$-case "ufc". Figure 6.3 shows that it is indeed worth calculating the full posterior distribution in order to save simulations. Finally, Figure 6.4 shows the relative frequency of correct selections and rankings in the above experiments. As it can be seen, it is always well above $1 - \alpha$, indicating that our setup is quite conservative.

6.3 The increasing μ-case

Next we look at the results for $\boldsymbol{\mu}$-case "inc", the results are quite similar. Figure 6.5 shows the CRN-case "isCRN" and again, $\mathcal{DPW}+$ performs best, though for the two first R&S-cases Best_1 and Best_{10}, GreedyOCBA has about the same performance.

Figure 6.6 again compares the result for $\mathcal{DPW}+$ for the estimators based on full posterior distributions and the ones using only marginal information. The

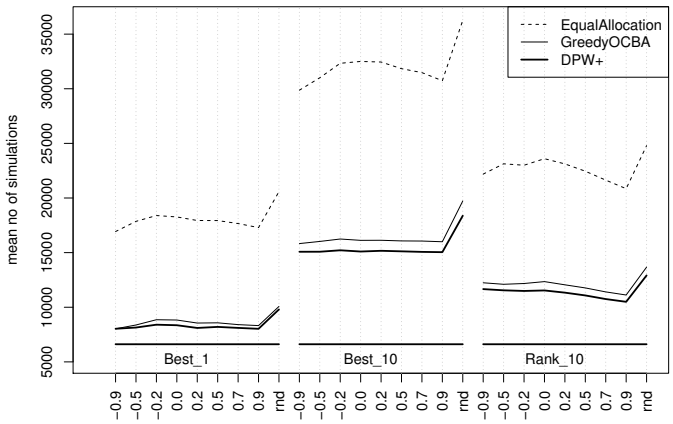

Figure 6.2: The unfavourable μ-case: comparison of the allocation strategies EqualAllocation, GreedyOCBA and $\mathcal{DPW}+$. Here, the posterior distribution is calculated using marginal distributions only.

advantage of the full distribution is obvious. The empirical PCS was well above 95% in all cases.

6.4 The uniform μ-case

In the "unif"-case, results are means over $M_\mu = 15$ different $\boldsymbol{\mu}$ drawn randomly from $[0, 100]^L$, over $M_{cov} = 15$ random covariance matrices and $M = 10$ repetitions. Results vary considerably depending on the difficulty of the random $\boldsymbol{\mu}$, so that the mean number of simulations gives only a rough picture of the performance.

Figure 6.7 shows that our new strategy $\mathcal{DPW}+$ is superior to the other strategies for positively correlated observations and with random covariance matrix, but it uses more simulations than GreedyOCBA for $cor < 0$. In Figure 6.8, it can be seen, that $\mathcal{DPW}+$ and GreedyOCBA have high empirical PCS except for one of the cases with $cor < 0$.

6.5 Comparison to the standard procedure $\mathcal{KN}$++

In Kim and Nelson [2006b] (see also Kim and Nelson [2006a]) the sequential procedure $\mathcal{KN}$++ is introduced. It is suitable to identify the best solution by iteratively excluding solutions that seem inferior to at least one of the other solutions.

In our tests, $\mathcal{KN}$++ needed much more simulation runs than our procedure BayesRS with allocation $\mathcal{DPW}+$, in particular in the $\boldsymbol{\mu}$-case "ufc", where $\mathcal{KN}$++ was not able to find the best solution within our limit of 150 000 simulations. To make results better comparable, we biased the setup in favor of $\mathcal{KN}$++. For $\mathcal{KN}$++ , we used a larger indifference zone parameter $\delta = 0.99$ in the $\boldsymbol{\mu}$-cases

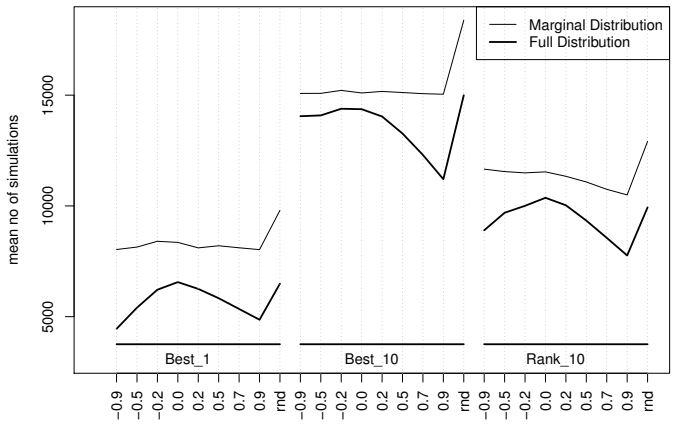

Figure 6.3: The unfavourable μ-case: comparison of the two CRN-cases for strategy $\mathcal{DPW}+$.

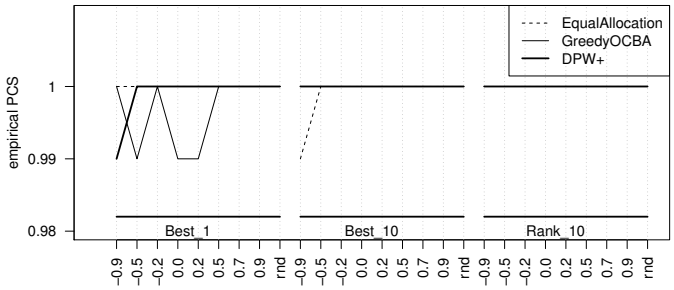

Figure 6.4: The unfavourable μ-case: the empirical frequency of correct selections in the above experiments.

"ufc" and "inc", and $\delta = 0.99\times$ the actual minimal distance in $\boldsymbol{\mu}$ for "unif"-case, thus adapting the parameter to the step between best and second best solution. For $\mathcal{DPW}+$, we used $\delta = 0.01$ for all $\boldsymbol{\mu}$-cases as before. Figure 6.9 shows the mean number of simulations needed for the R&S-case Best_1 and the three $\boldsymbol{\mu}$-cases. To make the figure better readable, we scaled down the results for $\mathcal{KN}++$ in the "unif"-case by a factor 10. In the $\boldsymbol{\mu}$-case "unif", we performed only $M = 5$ repetitions for $M_{cov} = 5$ covariance matrices and $M_\mu = 5$ different $\boldsymbol{\mu}$-values to save runtime.

With the relaxed indifference zone parameter $\delta = 0.99$, $\mathcal{KN}++$ was considerably faster than $\mathcal{DPW}+$ in the "ufc"-case, but missed the empirical PCS of 0.95 in most of these cases, as can be seen in Figure 6.10.

Hence, one may conclude that in most cases our new approach is superior to $\mathcal{KN}++$ with respect to the number of simulations needed and empirical error probabilities observed.

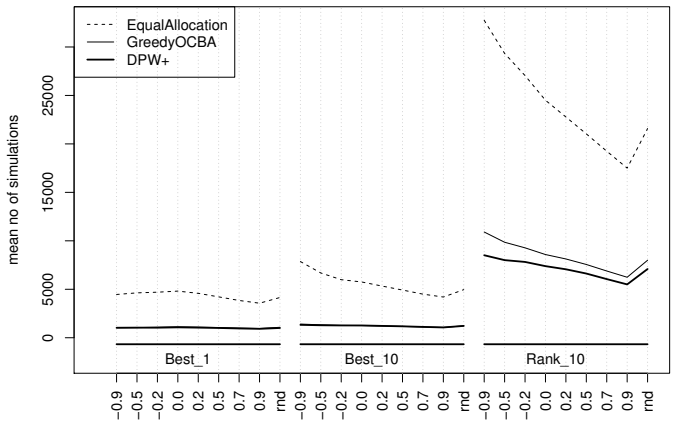

Figure 6.5: $\boldsymbol{\mu}$-case "inc": Comparison of the allocation strategies EqualAllocation, GreedyOCBA and $\mathcal{DPW}+$ using the full posterior distribution of the unknown means.

7 Conclusion and future work

In this paper we presented a new sequential Bayesian R&S procedure with support for common random numbers. Based on an approximation of the posterior distribution of the unknown mean and covariance, the simulation effort could be allocated to solutions in such a way that, empirically, a given PCS can be obtained with less simulations than are needed by other strategies.

In our future work we will extend this concept to multivariate selection problems. Essential parts of this problem were solved in Görder [2012].

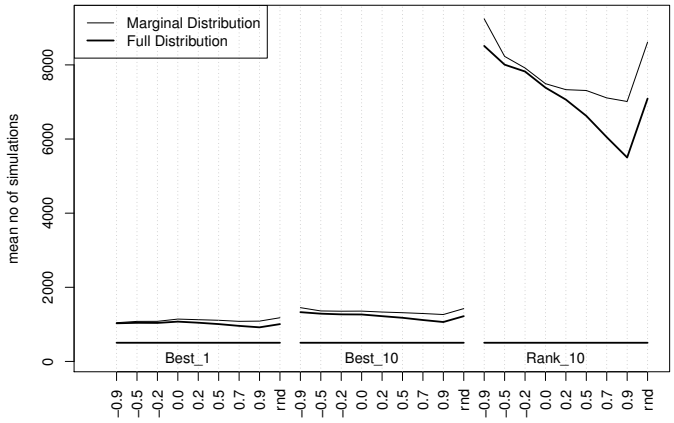

Figure 6.6: $\boldsymbol{\mu}$-case "inc": Comparison of the CRN-cases for the strategy $\mathcal{DPW}+$.

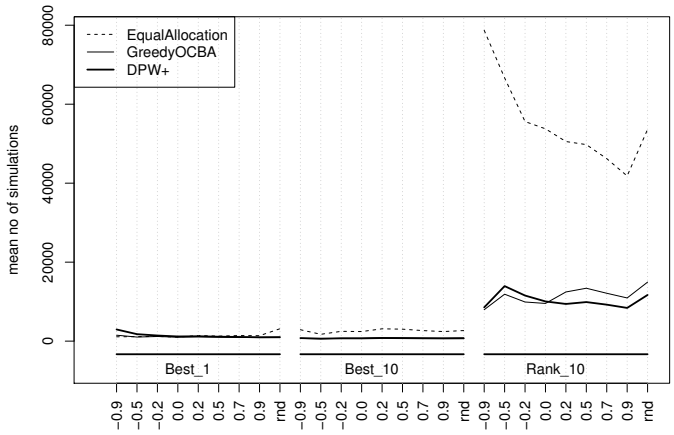

Figure 6.7: $\boldsymbol{\mu}$-case "unif": Comparison of the allocation strategies EqualAllocation, GreedyOCBA and $\mathcal{DPW}+$ using the full posterior distribution of the unknown means.

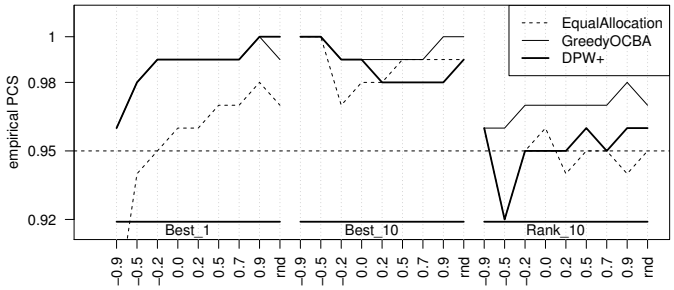

Figure 6.8: $\boldsymbol{\mu}$-case "unif": The empirical PCS.

A Derivation of the Posterior Distribution

We need the following well-known facts about multivariate Normal distributions, see e.g. Johnson et al. [2002] or DeGroot [2004], Sec. 5.4. Let $Y = (Y_1, \ldots, Y_d)$ be a random vector with distribution $N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Let $U := (Y_1, \ldots, Y_m)$ and $V := (Y_{m+1}, \ldots, Y_d)$ be a partition of Y for some $m < d$ and define

$$\begin{aligned}
\boldsymbol{\mu}_U &:= (\mu_1, \ldots, \mu_m), \quad \boldsymbol{\mu}_V := (\mu_{m+1}, \ldots, \mu_d) \quad \text{and} \\
\boldsymbol{\Sigma}_{UU} &:= \left(\sigma_{ij}\right)_{i,j=1,\ldots,m}, \quad \boldsymbol{\Sigma}_{VV} := \left(\sigma_{ij}\right)_{i,j=m+1,\ldots,d} \\
\boldsymbol{\Sigma}_{UV} &:= \left(\sigma_{ij}\right)_{\substack{i=1,\ldots,m \\ j=m+1,\ldots,d}}, \quad \boldsymbol{\Sigma}_{VU} := \left(\sigma_{ij}\right)_{\substack{i=m+1,\ldots,d \\ j=1,\ldots,m}}
\end{aligned}$$

so that

$$\boldsymbol{\mu} = (\boldsymbol{\mu}_U, \boldsymbol{\mu}_V) \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{UU} & \boldsymbol{\Sigma}_{UV} \\ \boldsymbol{\Sigma}_{VU} & \boldsymbol{\Sigma}_{VV} \end{pmatrix}.$$

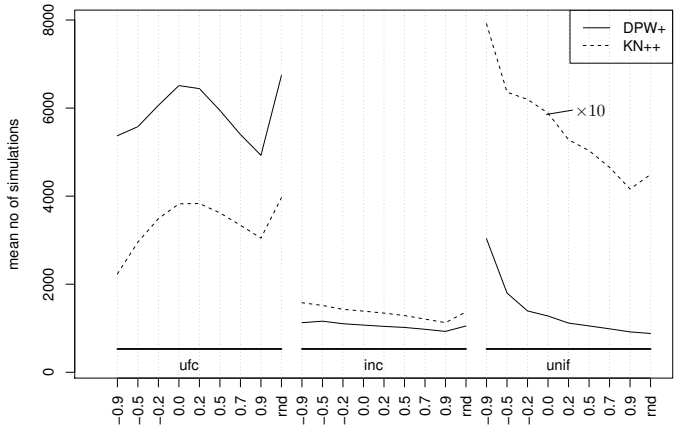

Figure 6.9: Comparison of $\mathcal{DPW}+$ and $\mathcal{KN}++$ for the R&S-case Best$_1$. Here, $\mathcal{KN}++$ has a larger indifference zone parameter δ for the first two cases and its "unif"-values are shown multiplied by 1/10.

Note that with the notation from (2.6), (2.7) we may write $\boldsymbol{\mu}_U = \boldsymbol{\mu}_{[<m+1]}$ and $\boldsymbol{\Sigma}_{UU} = \boldsymbol{\Sigma}_{[<m+1]}$. Then the marginal distributions of U and V are Normal:

$$U \sim \mathcal{N}_m(\boldsymbol{\mu}_U, \boldsymbol{\Sigma}_{UU}), \qquad V \sim \mathcal{N}_{d-m}(\boldsymbol{\mu}_V, \boldsymbol{\Sigma}_{VV}). \tag{A.1}$$

Moreover, the conditional distribution of V given $U = u$ is a $(d-m)$-dimensional Normal distribution $\mathcal{N}_{d-m}(\boldsymbol{\zeta}, \boldsymbol{\Gamma})$ with

$$\boldsymbol{\zeta} := \boldsymbol{\mu}_V + \boldsymbol{\Sigma}_{VU}\boldsymbol{\Sigma}_{UU}^{-1}(u - \boldsymbol{\mu}_U), \qquad \boldsymbol{\Gamma} := \boldsymbol{\Sigma}_{VV} - \boldsymbol{\Sigma}_{VU}\boldsymbol{\Sigma}_{UU}^{-1}\boldsymbol{\Sigma}_{UV}. \tag{A.2}$$

The converse does also hold: if U', V' are random variables such that U' has a $\mathcal{N}_m(\boldsymbol{\mu}_U, \boldsymbol{\Sigma}_{UU})$-distribution and the conditional distribution of V' given $U' = u'$ is as in (A.2), then the joint distribution of (U', V') is $\mathcal{N}_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

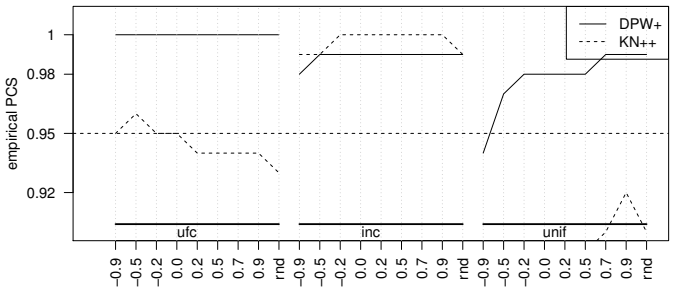

Figure 6.10: Comparison of the empirical PCS of $\mathcal{DPW}+$ and $\mathcal{KN}++$ for the R&S-case Best$_1$. Here, $\mathcal{KN}++$ was below 0.95 for most covariances in the $\boldsymbol{\mu}$-cases "ufc" and 'unif".

In particular, if $m = d-1$ so that $U = (Y_1, \ldots, Y_{d-1}), V = Y_d$, then we have $\boldsymbol{\mu}_V = \mu_d$, $\boldsymbol{\Sigma}_{VV} = \sigma_{dd}$ and

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{[<d]} & (\sigma_{1d}, \ldots, \sigma_{d-1,d})^T \\ (\sigma_{d1}, \ldots, \sigma_{d,d-1}) & \sigma_{dd} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Sigma}_{[<d]} & \boldsymbol{\Sigma}_{[d,<d]}^T \\ \boldsymbol{\Sigma}_{[d,<d]} & \sigma_{d,d} \end{pmatrix},$$

where we have used the symmetry of the covariance matrix $\boldsymbol{\Sigma}$ and the notation from (2.7). Then from (A.2), the conditional distribution of $V = Y_d$ given $U = (Y_1, \ldots, Y_{d-1}) = (y_1, \ldots, y_{d-1})$ is a one-dimensional Normal distribution with mean

$$\begin{aligned} \tilde{\mu}_{(d-1)}(y_1, \ldots, y_{d-1}) := \\ \mu_d + (\sigma_{d1}, \ldots, \sigma_{d,d-1}) \boldsymbol{\Sigma}_{[<d]}^{-1} \Big((y_1, \ldots, y_{d-1})^T - (\mu_1, \ldots, \mu_{d-1})^T \Big) \\ = \mu_d + \beta_d (\boldsymbol{y}_{[<d]} - \boldsymbol{\mu}_{[<d]}) \end{aligned} \tag{A.3}$$

and variance (independent of $\boldsymbol{y}$)

$$\begin{aligned} \tilde{\sigma}_{(d-1)} &:= \sigma_{dd} - (\sigma_{d1}, \ldots, \sigma_{d,d-1}) \boldsymbol{\Sigma}_{[<d]}^{-1} (\sigma_{d1}, \ldots, \sigma_{d,d-1})^T \\ &= \sigma_{dd} - \beta_d \boldsymbol{\Sigma}_{[<d]} \beta_d^T . \end{aligned} \tag{A.4}$$

For the **proof of Theorem 1** we first determine the likelihood function.

Theorem 2. Let $\boldsymbol{X}_{\cdot,k}, k = 1, 2, \ldots$ be i.i.d. $\mathcal{N}_L(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distributed with *known* covariance matrix $\boldsymbol{\Sigma}$ and unknown mean $\boldsymbol{\mu}$. Let the data $\boldsymbol{x} = \boldsymbol{x}_{\boldsymbol{n}} \in \mathcal{Z}_t$ with $\boldsymbol{n} = (n_1, \ldots, n_L)$, $n_1 \geq n_2 \geq \cdots \geq n_L$ for some $\boldsymbol{t} \in \mathbb{N}$ be given.

Then the likelihood function of the unknown mean $\boldsymbol{\mu}$ given data $\boldsymbol{x}$ is

$$l(\boldsymbol{\mu}, \boldsymbol{x}) \quad \propto \quad \phi_1(\mu_1;\ \bar{\boldsymbol{x}}_1, \sigma_{11}/n_1) \cdot \prod_{i=2}^{L} \phi_1(\mu_i;\ \bar{\boldsymbol{x}}_i + \beta_i(\boldsymbol{\mu}_{[<i]} - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}), \frac{\tilde{\sigma}_{(i-1)}}{n_i}) \tag{A.5}$$

where $\phi_1(\cdot\ ; a, b)$ is the one-dimensional Normal density with mean a and variance b.

Proof of Theorem 2. As we assume that the covariance matrix $\boldsymbol{\Sigma}$ is known, the likelihood function for $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_L)$, given the sample $\boldsymbol{x} = \boldsymbol{x}_{(n_1, \ldots, n_L)}$ as in (2.4) can be written as a product of independent blocks of Normal densities of different dimensionality. Let

$$l_i := \max\{l \mid l \in \{1, \ldots, L\} \text{ such that } n_l = n_i\}, \qquad i = 1, \ldots, L \tag{A.6}$$

be the number of solutions with at least n_i observations. l_i is the 'height' of the data blocks with at least n_i observations, see Fig. A.1. Then with $n_{L+1} := 0$ we have for the likelihood function

$$l(\boldsymbol{\mu}; \boldsymbol{x}) = \prod_{i=1}^{L} \prod_{k=n_{i+1}+1}^{n_i} \phi_{l_i}\big((x_{1,k}, \ldots, x_{l_i,k});\ \boldsymbol{\mu}_{[\leq l_i]}, \boldsymbol{\Sigma}_{[\leq l_i]}\big), \tag{A.7}$$

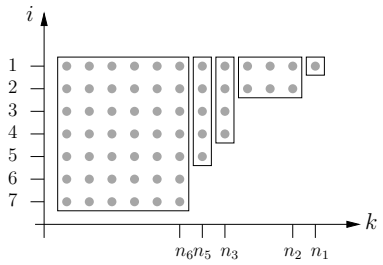

Figure A.1: The sample from Fig. 2.2 has $l_1 = 1, l_2 = 2, l_3 = l_4 = 4, l_5 = 5, l_6 = l_7 = 7$.

where ϕ_l is the density function of the l-dimensional normal distribution. Here, the inner product describes the likelihood for the sample values within one of the blocks as marked in Fig. A.1. Note that (A.7) may contain empty products (defined to be 1) if $n_i = n_{i+1}$. Now each of the l_i-dimensional densities in (A.7) can be factorized into l_i factors of one-dimensional conditional densities. We write $f_{Y|Z}(\cdot|z)$ for the density of the conditional distribution of Y given $Z = z$. For $i \in \{1, \dots, L\}$ let $n_{i+1} + 1 \leq k \leq n_i$, then using (A.3) and (A.4) we obtain

$$\begin{aligned}
&\phi_{l_i}\big((x_{1k}, \dots, x_{l_ik}); \boldsymbol{\mu}_{[\leq l_i]}, \boldsymbol{\Sigma}_{[\leq l_i]}\big) \\
&\quad = f_{X_{1k}}(x_{1k}) \cdot f_{X_{2k}|X_{1k}}(x_{2k}|x_{1k}) \cdot \dots \\
&\qquad\qquad \cdot f_{X_{l_ik}|X_{1,k},\dots,X_{l_i-1k}}(x_{l_ik}|x_{1k}, \dots, x_{l_i-1k}) \\
&\quad = \phi_1(x_{1k};\ \mu_1, \sigma_{11}) \cdot \phi_1(x_{2k};\ \tilde{\mu}_{(1)}(x_{1k}), \tilde{\sigma}_{(1)}) \cdot \dots \\
&\qquad\qquad \cdot \phi_1\big(x_{l_ik};\ \tilde{\mu}_{(l_i-1)}(x_{1k}, \dots, x_{l_i-1,k}), \tilde{\sigma}_{(l_i-1)}\big) \\
&\quad = \phi_1(x_{1k};\ \mu_1, \sigma_{11}) \cdot \phi_1(x_{2k};\ \tilde{\mu}_{(1)}(\boldsymbol{x}_{[<2,k]}), \tilde{\sigma}_{(1)}) \cdot \dots \\
&\qquad\qquad \cdot \phi_1\big(x_{l_ik};\ \tilde{\mu}_{(l_i-1)}(\boldsymbol{x}_{[<l_i,k]}), \tilde{\sigma}_{(l_i-1)}\big)
\end{aligned} \tag{A.8}$$

where $\boldsymbol{x}_{[<i,k]} := (x_{1k}, \dots, x_{i-1,k})^T$. Plugging (A.8) into (A.7) and reordering terms we get

$$l(\boldsymbol{\mu}; \boldsymbol{x}) = \prod_{j=1}^{n_1} \phi_1(x_{1j};\ \mu_1, \sigma_{11}) \cdot \prod_{i=2}^{L} \prod_{j=1}^{n_i} \phi_1(x_{ij};\ \tilde{\mu}_{(i-1)}(\boldsymbol{x}_{[<i,j]}), \tilde{\sigma}_{(i-1)}). \tag{A.9}$$

Dropping terms that do not depend on $\boldsymbol{\mu}$ (remember that $\boldsymbol{\Sigma}$ was assumed to be known) we obtain from straightforward calculations

$$\prod_{j=1}^{n_1} \phi_1(x_{1j};\ \mu_1, \sigma_{11}) \propto \phi_1(\bar{\boldsymbol{x}}_1;\ \mu_1, \sigma_{11}/n_1) \qquad \text{and} \tag{A.10}$$

$$\prod_{j=1}^{n_i} \phi_1(x_{ij};\ \tilde{\mu}_{(i-1)}(\boldsymbol{x}_{[<i,j]}), \tilde{\sigma}_{(i-1)}) \propto \\ \phi_1(\bar{\boldsymbol{x}}_i;\ \mu_i + \beta_i(\bar{\boldsymbol{x}}^{(n_i)}_{[<i]} - \boldsymbol{\mu}_{[<i]}), \tilde{\sigma}_{(i-1)}/n_i) \tag{A.11}$$

for $i = 2, \ldots, L$. From (A.9), (A.10) and (A.11) we therefore obtain

$$\begin{aligned} l(\boldsymbol{\mu}, \boldsymbol{x}) &\propto \phi_1(\bar{\boldsymbol{x}}_1;\ \mu_1, \sigma_{11}/n_1) \cdot \prod_{i=2}^{L} \phi_1(\bar{\boldsymbol{x}}_i;\ \mu_i + \beta_i(\bar{\boldsymbol{x}}_{[<i]}^{(n_i)} - \boldsymbol{\mu}_{[<i]}), \tilde{\sigma}_{(i-1)}/n_i) \\ &= \phi_1(\mu_1;\ \bar{\boldsymbol{x}}_1, \sigma_{11}/n_1) \cdot \prod_{i=2}^{L} \phi_1(\mu_i;\ \bar{\boldsymbol{x}}_i + \beta_i(\boldsymbol{\mu}_{[<i]} - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}), \tilde{\sigma}_{(i-1)}/n_i). \end{aligned} \tag{A.12}$$

□

Proof of Theorem 1. Using the uninformative prior $\pi(\boldsymbol{\mu}) = 1$ with $\boldsymbol{\Sigma}$ fixed, we see that (A.12) is in fact the posterior density for $W = \boldsymbol{\mu}$ given $\boldsymbol{X} = \boldsymbol{x}$ (up to constants that do not depend on $\boldsymbol{\mu}$).

Moreover, from (A.2) we see, that (A.12) is the factorized representation of a L-dimensional Normal density $\phi_L(\boldsymbol{\mu};\ \boldsymbol{\nu}, \boldsymbol{\Lambda})$ where the mean $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_L)$ and covariance matrix $\boldsymbol{\Lambda}$ are such that the operations in (A.2) lead to the representation in (A.12). To find $\boldsymbol{\nu}$ and $\boldsymbol{\Lambda}$ we have to undo the operations from (A.2). This is possible since we see from (A.12) that

$$f_{W_1|\boldsymbol{X}}(\mu_1 \mid \boldsymbol{x}) = \phi_1(\mu_1;\ \bar{\boldsymbol{x}}_1, \sigma_{11}/n_1) \tag{A.13}$$

$$f_{W_i|\boldsymbol{X}, W_1, \ldots, W_{i-1}}(\mu_i \mid \boldsymbol{x}, \mu_1, \ldots, \mu_{i-1}) = \phi_1(\mu_i;\ \bar{\boldsymbol{x}}_i + \beta_i(\boldsymbol{\mu}_{[<i]} - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}), \tilde{\sigma}_{(i-1)}/n_i). \tag{A.14}$$

From this it is also obvious, that

$$\begin{aligned} f_{W_1|\boldsymbol{X}}(\mu_1 \mid \boldsymbol{x}) &= f_{W_1|\boldsymbol{X}_{1,\cdot}}(\mu_1 \mid \boldsymbol{x}_{1\cdot}) \quad \text{and} \\ f_{W_i|\boldsymbol{X}, W_1, \ldots, W_{i-1}}(\mu_1 \mid \boldsymbol{x}, \mu_1, \ldots, \mu_{i-1}) &= f_{W_i|\boldsymbol{X}_{[<i,\cdot]}, W_{[<i]}}(\boldsymbol{\mu}_{[<i]} \mid \boldsymbol{x}_{[<i,\cdot]}) \end{aligned}$$

where $\boldsymbol{x}_{1\cdot} = (x_{11}, x_{12}, \ldots, x_{1n_1})$ and $\boldsymbol{x}_{[<i,\cdot]}$ denotes all observations for solutions $j = 1, \ldots, i-1$. This means that the conditional expressions do not depend on observations for solutions $j > 1$ resp. $j \geq i$. Therefore we can conclude for the means $\nu_1, \ldots, \nu_L$

$$\nu_1 = \mathbf{E}[W_1 \mid \boldsymbol{X} = \boldsymbol{x}] = \mathbf{E}[W_1 \mid \boldsymbol{X}_{1\cdot} = \boldsymbol{x}_{1\cdot}] = \bar{\boldsymbol{x}}_1 \tag{A.15}$$

$$\begin{aligned} \nu_i = \mathbf{E}[W_i \mid \boldsymbol{X} = \boldsymbol{x}] &= \mathbf{E}[W_i \mid \boldsymbol{X}_{[\leq i,\cdot]} = \boldsymbol{x}_{[\leq i,\cdot]}] \\ &= \mathbf{E}\Big[\mathbf{E}[W_i \mid \boldsymbol{X}_{[\leq i,\cdot]}, W_{[<i]}] \;\Big|\; \boldsymbol{X}_{[\leq i,\cdot]} = \boldsymbol{x}_{[\leq i,\cdot]}\Big] \\ &= \mathbf{E}\Big[\bar{\boldsymbol{x}}_i + \beta_i(W_{[<i]} - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}) \;\Big|\; \boldsymbol{X}_{[\leq i,\cdot]} = \boldsymbol{x}_{[\leq i,\cdot]}\Big] \\ &= \bar{\boldsymbol{x}}_i + \beta_i\Big(\mathbf{E}\Big[W_{[<i]} \;\Big|\; \boldsymbol{X}_{[\leq i,\cdot]} = \boldsymbol{x}_{[\leq i,\cdot]}\Big] - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}\Big) \\ &= \bar{\boldsymbol{x}}_i + \beta_i(\boldsymbol{\nu}_{[<i]} - \bar{\boldsymbol{x}}_{[<i]}^{(n_i)}) \qquad \text{for } i = 2, \ldots, L. \end{aligned} \tag{A.16}$$

For the $(L \times L)$ posterior covariance matrix

$$\boldsymbol{\Lambda} := \operatorname{cov}[W \mid \boldsymbol{X} = \boldsymbol{x}] = \Big(\operatorname{cov}[W_k, W_l \mid \boldsymbol{X} = \boldsymbol{x}]\Big)_{k,l=1,\ldots,L}$$

we again put

$$\mathbf{\Lambda}_{[\le i]} := \Big(\mathrm{cov}[W_k, W_l \mid \boldsymbol{X} = \boldsymbol{x}]\Big)_{k,l=1,\dots,i}.$$

Then we have for $i \ge 2$ that $\mathbf{\Lambda}_{[\le i]}$ equals

$$\left(\begin{array}{c|c} \mathbf{\Lambda}_{[<i]} & \begin{array}{c}\mathrm{cov}[W_1, W_i|\boldsymbol{X}=\boldsymbol{x}]\\ \vdots \\ \mathrm{cov}[W_{i-1}, W_i|\boldsymbol{X}=\boldsymbol{x}]\end{array} \\ \hline \mathrm{cov}[W_i, W_1|\boldsymbol{X}=\boldsymbol{x}] \ \dots \ \mathrm{cov}[W_i, W_{i-1}|\boldsymbol{X}=\boldsymbol{x}] & \mathrm{cov}[W_i, W_i|\boldsymbol{X}=\boldsymbol{x}] \end{array}\right) \tag{A.17}$$

To determine the entries of this matrix, we use the following facts about the conditional covariance which are straightforward to prove. Let U, V, Z and Y be random variables such that all integrals exist and let g be a suitable function :

$$\begin{aligned}
\mathrm{cov}[U, V \mid Z] &= \mathbf{E}[U \cdot V \mid Z] - \mathbf{E}[U \mid Z] \cdot \mathbf{E}[V \mid Z], \\
\mathrm{cov}\Big[U, \Big(V + g(Z)\Big) \mid Z\Big] &= \mathrm{cov}[U, V \mid Z], \\
\mathrm{cov}[U, V \mid Z] &= \mathrm{cov}\Big[U,\ \mathbf{E}[V \mid Y, Z] \,\Big|\, Z\Big] \quad \text{if } U = g(Y), \qquad \text{(A.18)} \\
\mathrm{cov}[U, U \mid Z] &= \boldsymbol{V}[U \mid Z] \qquad \text{(A.19)} \\
&= \mathbf{E}\Big[\boldsymbol{V}[U \mid Z, Y] \,\Big|\, Z\Big] + \boldsymbol{V}\Big[\mathbf{E}[U \mid Z, Y] \,\Big|\, Z\Big].
\end{aligned}$$

We now have from (A.13)

$$\begin{aligned}
\mathbf{\Lambda}_{[\le 1]} &= \mathrm{cov}[W_1, W_1 \mid \boldsymbol{X} = \boldsymbol{x}] \\
&= \boldsymbol{V}[W_1 \mid \boldsymbol{X} = \boldsymbol{x}] = \frac{\sigma_{11}}{n_1} = \mathrm{cov}[W_1, W_1 \mid \boldsymbol{X}_1. = \boldsymbol{x}_1.] \qquad \text{(A.20)}
\end{aligned}$$

and similarly from (A.14) and (A.19)

$$\begin{aligned}
\mathrm{cov}[W_i, W_i \mid \boldsymbol{X} = \boldsymbol{x}] &= \boldsymbol{V}[W_i \mid \boldsymbol{X} = \boldsymbol{x}] \\
&= \mathbf{E}\Big[\boldsymbol{V}[W_i|\boldsymbol{X}, W_{[<i]}] \,\Big|\, \boldsymbol{X} = \boldsymbol{x}\Big] + \boldsymbol{V}\Big[\mathbf{E}[W_i \mid \boldsymbol{X}, W_{[<i]}] \,\Big|\, \boldsymbol{X} = \boldsymbol{x}\Big] \qquad \text{(A.21)} \\
&= \mathbf{E}\Big[\frac{\tilde{\sigma}_{(i-1)}}{n_i} \,\Big|\, \boldsymbol{X} = \boldsymbol{x}\Big] \\
&\qquad + \boldsymbol{V}\Big[\bar{X}_i + \beta_i(W_{[<i]} - \bar{X}_i^{(n_i)}) \,\Big|\, \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \\
&= \frac{\tilde{\sigma}_{(i-1)}}{n_i} + \boldsymbol{V}\Big[\beta_i W_{[<i]} \,\Big|\, \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \\
&= \frac{1}{n_i}(\sigma_{ii} - \beta_i \mathbf{\Sigma}_{[<i]} \beta_i^T) + \beta_i \ \mathrm{cov}\big[W_{[<i]} \mid \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\big] \ \beta_i^T \\
&= \frac{1}{n_i}(\sigma_{ii} - \beta_i \mathbf{\Sigma}_{[<i]} \beta_i^T) + \beta_i \ \mathbf{\Lambda}_{[<i]} \ \beta_i^T.
\end{aligned}$$

Finally, for $1 \leq k \leq i-1$, we have using (A.18) and (A.14)

$$\begin{aligned}
\operatorname{cov}\Big[W_k, W_i \;\Big|\; \boldsymbol{X} = \boldsymbol{x}\Big] &= \operatorname{cov}\Big[W_k, W_i \;\Big|\; \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \qquad \text{(A.22)} \\
&= \operatorname{cov}\Big[W_k,\ \mathbf{E}[W_i \mid W_{[<i]}, \boldsymbol{X}_{[\leq i]}] \;\Big|\; \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \\
&= \operatorname{cov}\Big[W_k,\ \bar{X}_i + \beta_i(W_{[<i]} - \bar{\boldsymbol{X}}^{(n_i)}_{[<i]}) \;\Big|\; \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \\
&= \operatorname{cov}\Big[W_k,\ \beta_i W_{[<i]} \;\Big|\; \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}\Big] \\
&= \beta_i \Big(\operatorname{cov}[W_k, W_l \;|\; \boldsymbol{X}_{[<i,\cdot]} = \boldsymbol{x}_{[<i,\cdot]}]\Big)^T_{l=1,\ldots,i-1} \\
&= \beta_i\ \boldsymbol{\Lambda}_{[<i]}.
\end{aligned}$$

From (A.20) - (A.22) and (A.17) we now obtain the recursion

$$\boldsymbol{\Lambda}_{[\leq 1]} = \frac{\sigma_{11}}{n_1}, \qquad \boldsymbol{\Lambda}_{[\leq i]} = \left(\begin{array}{c|c} \boldsymbol{\Lambda}_{[<i]} & \boldsymbol{\Lambda}_{[<i]}\ \beta_i^T \\ \hline \beta_i\ \boldsymbol{\Lambda}_{[<i]} & \frac{1}{n_i}(\sigma_{ii} - \beta_i \boldsymbol{\Sigma}_{[<i]} \beta_i^T) + \beta_i\ \boldsymbol{\Lambda}_{[<i]}\ \beta_i^T \end{array}\right) \qquad \text{(A.23)}$$

for $i = 2, \ldots, L$, which concludes the Proof of Theorem 1. □

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