Bootstrap tuning in ordered model selection

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Abstract

In the problem of model selection for a given family of linear estimators, ordered by their variance, we offer a new “smallest accepted” approach motivated by Lepski’s method and multiple testing theory. The procedure selects the smallest model which satisfies an acceptance rule based on comparison with all larger models. The method is completely data-driven and does not use any prior information about the variance structure of the noise: its parameters are adjusted to the underlying possibly heterogeneous noise by the so-called “propagation condition” using a wild bootstrap method. The validity of the bootstrap calibration is proved for finite samples with an explicit error bound. We provide a comprehensive theoretical study of the method and describe in detail the set of possible values of the selector $\hat{m}$. We also establish some precise oracle error bounds for the corresponding estimator $\hat{\theta} = \hat{\theta}_{\hat{m}}$ which equally applies to estimation of the whole parameter vectors, some subvector or linear mapping, as well as the estimation of a linear functional.

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1 Introduction

Model selection is one of the key topics in mathematical statistics. A choice between models of differing complexity can often be viewed as a trade-off between overfitting the data by choosing a model which has too many degrees of freedom and smoothing out the underlying structure in the data by choosing a model which has too few degrees of freedom. This trade-off which shows up in most methods as the classical bias-variance trade-off is at the heart of every model selection method (as for example in unbiased risk estimation, Kneip (1994) or in penalized model selection, Barron et al. (1999), Massart (2007)). This is also the case in Lepski’s method, Lepski (1990), Lepski (1991), Lepski (1992), Lepski and Spokoiny (1997), Lepski et al. (1997), Birgé (2001) and risk hull minimization, Cavalier and Golubev (2006). Many of these methods allow their strongest theoretical results only for highly idealized situations (for example sequence space models), are very specific to the type of problem under consideration (for instance, signal or functional estimation), require to know the noise behavior (like homogeneity) and the exact noise level. Moreover, they typically involve an unwieldy number of calibration constants whose choice is crucial to the applicability of the method and is not addressed by the theoretical considerations. For instance, any Lepski-type method requires to fix a numerical constant in the definition of the threshold, the theoretical results only apply if this constant is sufficiently large while the numerical results benefit from the choice of a rather small constant. Spokoiny and Vial (2009) offered a propagation approach to calibration of Lepski’s method in the case of the estimation of a one-dimensional quantity of interest. However, the proposal still requires the exact knowledge of the noise level and only applies to linear functional estimation. A similar approach has been applied to local constant density estimation with sup-norm risk in Gach et al. (2013) and to local quantile estimation in Spokoiny et al. (2013).

In the case of unknown but homogeneous noise, generalized cross validation can be used instead of unbiased risk estimation method. For the penalized model selection, recently a number of proposals appeared to apply one or another resampling method. Arlot (2009) suggested the use of resampling methods for the choice of an optimal penalization, following the framework of penalized model selection, Barron et al. (1999), Birgé and Massart (2007). The validity of a bootstrapping procedure for Lepski’s method has also been studied in Chernozhukov et al. (2014) with new innovative technical tools with applications to honest adaptive confidence bands.

An alternative approach to adaptive estimation is based on aggregation of different estimates; see Goldenshluger (2009) and Dalalyan and Salmon (2012) for an overview of the existing results. However, the proposed aggregation procedures either require
two independent copies of the data or involves a data splitting for estimating the noise variance. Each of these requirements is very restrictive for practical applications.

Another point to mention is that the majority of the obtained results on adaptive estimation focus on the quality of estimating the unknown response, that is, the loss is measured by the difference between the true response and its estimate. At the same time, inference questions like confidence estimation would require to know some additional information about the right model parameter. Only few results address the issue of estimating the true (oracle) model. Moreover, there are some negative results showing that a construction of adaptive honest confidence sets is impossible without special conditions like self-similarity; see, e.g. Gine and Nickl (2010).

This paper aims at developing a unified approach to the problem of ordered model selection with the focus on the quality of model selection rather than on accuracy of adaptive estimation under realistic assumptions on the model. Our setup covers linear regression and linear inverse problems, and equally applies to estimation of the whole parameter vectors, a subvector or linear mapping, as well as estimation of a linear functional. The proposed procedure and the theoretical study are also unified and do not distinguish between models and problems. In the case of a linear inverse problem, it is applicable to mild and severely ill-posed problems without prior knowledge of the type and degree of ill-posedness; cf. Tsybakov (2000), Cavalier et al. (2002). Another important issue is that the procedure does not use any prior information about the variance structure of the noise under assumption of minimal Hölder smoothness $1/4$ on the underlying function. The method automatically adjusts the parameters to the underlying possibly heterogeneous noise: the resampling technique allows to achieve the same quality of estimation as if the noise structure were precisely known. Also we allow for a model misspecification: the linear structure of the response can be violated, in this case the procedure adaptively recovers the best linear projection.

Consider a linear model $Y = \Psi^\top \theta^* + \varepsilon$ in $\mathbb{R}^n$ for an unknown parameter vector $\theta^* \in \mathbb{R}^p$ and a given $p \times n$ design matrix $\Psi$. Suppose that a family of linear smoothers $\tilde{\theta}_m = S_m Y$ is given, where $S_m$ is for each $m \in M$ a given $p \times n$ matrix. We also assume that this family is ordered by the complexity of the method. The task is to develop a data-based model selector $\hat{m}$ which performs nearly as good as the optimal choice, which depends on the model and is not available. The proposed procedure called the “smallest accepted” (SmA) rule can be viewed as a calibrated Lepski-type method. The idea how the parameters of the method can be tuned, originates from Spokoiny and Vial (2009) and is related to a multiple testing problem. The whole procedure is based on family of pairwise tests, each model is tested against all larger ones. Finally the smallest accepted model is selected. The critical values for this multiple testing procedure are fixed using
the so-called propagation condition. Theorem 2.1 presents finite sample results on the behavior of the proposed selector \( \hat{m} \) and the corresponding estimator \( \hat{\theta} = \tilde{\theta}_{\hat{m}} \). In particular, it describes a concentration set \( M^0 \) for the selected index \( \hat{m} \) and states an oracle bound for the resulting estimator \( \hat{\theta} = \tilde{\theta}_{\hat{m}} \). Usual rate results can be easily derived from these statements. Further results address the important issue called “the payment for adaptation” which can be defined as the gap between oracle and adaptive bounds. Theorem 2.2 gives a general description of this quantity. Then we specify the results to important special cases like projection estimation and estimation of a linear functional. It appears, that in some cases the obtained results yield sharp asymptotic bounds. In some other cases they lead to the usual log-price for adaptation. However, all these results require a known noise distribution. Section 3 explains how the proposed procedure can be tuned in the case of unknown noise using a bootstrap procedure. We establish explicit error bounds on the accuracy of the bootstrap approximation and show that the procedure with bootstrap tuning does essentially the same job as the ideal procedure designed for the known noise. The study is quite involved because the procedure uses the same data twice for parameter tuning and for model selection.

The paper is structured as follows. The next section presents the procedure and the results for an idealistic situation when the noise distribution is precisely known. We introduce the SmA selector \( \hat{m} \) and explain how it can be calibrated. Then we describe the set of possible \( \hat{m} \)-values and establish probabilistic oracle bounds. Section 2.6 explains how the method and the results can be extended to the case of a polynomial loss function. The results are also specified to the particular problems of projection and linear functional estimation. Section 3 extends the method and the study to the realistic case with unknown heteroscedastic noise by using a resampling technique. The proofs and a detailed study of the bootstrap procedure in the linear Gaussian setup are given in the appendix. We also collect there some useful technical statements for Gaussian quadratic forms and sums of random matrices.

2 Model and problem. Known noise variance

This section presents the model selector for the idealistic case when the noise distribution is precisely known. In the next section we explain how the unknown noise structure can be recovered from the data using a resampling technique. First we specify our setup. We consider the following linear Gaussian model:

\[
Y_i = \Psi_i^\top \theta^* + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2) \quad \text{i.i.d.}, \quad i = 1, \ldots, n, \tag{2.1}
\]
with given design $\Psi_1, \ldots, \Psi_n$ in $\mathbb{R}^p$. We also write this equation in vector form $Y = \Psi^\top \theta^* + \varepsilon \in \mathbb{R}^n$, where $\Psi$ is $p \times n$ design matrix and $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$. Below we assume a deterministic design, otherwise one can understand the results conditioned on the design realization.

In what follows, we allow the model (2.1) to be completely misspecified. We mainly assume that the observations $Y_i$ are independent and define the response vector $f^* = \mathbb{E} Y$ with entries $f_i$. Such a model can be written as

$$ Y_i = f_i + \varepsilon_i. \quad (2.2) $$

Our study allows that the linear parametric assumption $f^* = \Psi^\top \theta^*$ is violated, and the underlying noise $\varepsilon = (\varepsilon_i)$ can be heterogeneous and non-Gaussian. However, in this section we assume the noise distribution to be known. The main oracle results of Theorem 2.1 below do not require any further conditions on the noise. Some upper bounds on the quantities $\zeta_{m^*}$ entering in the oracle bounds are established under i.i.d. Gaussian noise, but can be easily extended to non-Gaussian heterogeneous noise under moment conditions. For the linear model (2.2), define $\theta^* \in \mathbb{R}^p$ as the vector providing the best linear fit:

$$ \theta^* \overset{\text{def}}{=} \arg\min_{\theta} \mathbb{E}\|Y - \Psi^\top \theta\|^2 = (\Psi \Psi^\top)^{-1} \Psi f^*. $$

As usual, a pseudo-inversion is assumed if the matrix $\Psi \Psi^\top$ is degenerated.

Below we assume a family $\{\tilde{\theta}_m\}$ of linear estimators $\tilde{\theta}_m = S_m Y$ of $\theta^*$ to be given. Typical examples include projection estimation on an $m$-dimensional subspace or regularized estimation with a regularization parameter $\alpha_m$, penalized estimators with a quadratic penalty function, etc. To include specific problems like subvector-functional estimation, we also introduce a weighting $q \times p$-matrix $W$ for some fixed $q \geq 1$ and define quadratic loss and risk with this weighting matrix $W$:

$$ \varrho_m \overset{\text{def}}{=} \|W(\tilde{\theta}_m - \theta^*)\|^2, \quad R_m \overset{\text{def}}{=} \mathbb{E}\|W(\tilde{\theta}_m - \theta^*)\|^2. $$

Of course, the loss and the risk depend on the choice of $W$. We do not indicate this dependence explicitly but it is important to keep in mind the role of $W$ in the definition of $\varrho_m$. Typical examples of $W$ are as follows.

**Estimation of the whole vector $\theta^*$** Let $W$ be the identity matrix $W = I_p$ with $q = p$. This means that the estimation loss is measured by the usual squared Euclidean norm $\|\tilde{\theta}_m - \theta^*\|^2$. 


Prediction Let $W$ be the square root of the total Fisher information matrix $\mathbb{F} = \sigma^{-2} \Psi \Psi^\top$, that is, $W^2 = \mathbb{F}$. Such a type of loss is usually referred to as prediction loss because it measures the fit and the prediction ability of the true model by the model with the parameter $\theta$.

Semiparametric estimation Let the target of estimation not be the whole vector $\theta^*$ but some subvector $\theta_0^*$ of dimension $q$. The estimate $\Pi \tilde{\theta}_m$ is called the profile maximum likelihood estimate. The matrix $W$ can be defined as the projector $\Pi_0$ on the $\theta_0^*$ subspace. The corresponding loss is equal to the squared Euclidean norm in this subspace:

$$\varrho_m = \|\Pi_0 (\tilde{\theta}_m - \theta^*)\|^2.$$

Alternatively, one can select $W^2$ as the efficient Fisher information matrix defined by the relation

$$W^2 \overset{\text{def}}{=} \mathbb{F} = (\Pi_0 \mathbb{F} \Pi_0^\top)^{-1}.$$

Linear functional estimation The choice of the weighting matrix $W$ can be adjusted to address the problem of estimating some functionals of the whole parameter $\theta^*$. In all cases, the most important feature of the estimators $\tilde{\theta}_m$ is linearity. It greatly simplifies the study of their properties including the prominent bias-variance decomposition of the risk of $\tilde{\theta}_m$. Namely, for the model (2.2) with $\mathbb{E}\varepsilon = 0$, it holds

$$\mathbb{E}\tilde{\theta}_m = \theta_m^* = S_m f^*,
\mathcal{R}_m = \|W(\theta_m^* - \theta^*)\|^2 + \text{tr}\{WS_m \text{Var}(\varepsilon) S_m^\top W^\top\}
= \|W(S_m - S) f^*\|^2 + \text{tr}\{WS_m \text{Var}(\varepsilon) S_m^\top W^\top\}.$$

(2.3)

The optimal choice of the parameter $m$ can be defined by risk minimization:

$$m^* \overset{\text{def}}{=} \arg\min_{m \in \mathcal{M}} \mathcal{R}_m.$$

The model selection problem can be described as the choice of $m$ by data which mimics the oracle, that is, we aim at constructing a selector $\hat{m}$ leading to the adaptive estimate $\hat{\theta} = \tilde{\theta}_{\hat{m}}$ with properties similar to the oracle estimate $\tilde{\theta}_m^*$. Below we discuss the ordered case. The parameter $m \in \mathcal{M}$ is treated as complexity of the method $\tilde{\theta}_m$. In some cases the set $\mathcal{M}$ of possible $m$ choices can be countable and/or continuous and even unbounded. For simplicity of presentation, we assume that
$M$ is a finite set of positive numbers, $|M|$ stands for its cardinality. Typical examples are given by the number of terms in the Fourier expansion, or by the bandwidth in the kernel smoothing. In general, complexity can be naturally expressed via the variance of the stochastic term of the estimator $\tilde{\theta}_m$: the larger $m$, the larger is the variance $\text{Var}(W\tilde{\theta}_m)$. In the case of projection estimation with $m$-dimensional projectors $S_m$, this variance is linear in $m$, $\text{Var}(\tilde{\theta}_m) = \sigma^2 m$. In general, dependence of the variance term on $m$ may be more complicated but the monotonicity constraint (2.4) has to be preserved.

Further, it is implicitly assumed that the bias term $\|W(\theta^* - \theta^*_m)\|^2$ becomes small when $m$ increases. The smallest index $m = m_0$ corresponds to the simplest (zero) model with probably a large bias, while $m$ large ensures a good approximation quality $\theta^*_m \approx \theta^*$ and a small bias at cost of a big complexity measured by the variance term. In the case of projection estimation, the bias term in (2.3) describes the accuracy of approximating the response $f^*$ by an $m$-dimensional linear subspace and this approximation improves as $m$ grows. However, in general, in contrast to the case of projection estimation, one cannot require that the bias term $\|W(\theta^* - \theta^*_m)\|$ monotonously decreases with $m$. One example is given by an estimation-at-a-point problem.

**Example 2.1.** Suppose that a signal $\theta^*$ is observed with noise: $Y_i = \theta^*_j + \varepsilon_j$. Consider the set of projection estimates $\tilde{\theta}_m$ on the first $m$ coordinates and the target is $\phi^* \overset{\text{def}}{=} W\theta = \sum_j \theta_j$. If $\theta^*$ is composed of alternating blocks of 1’s and -1’s with equal length, then the bias $|\phi^* - \phi^*_m|$ for $\phi^*_m = \sum_{j \leq m} \theta^*_j$ is not monotonous in $m$.

### 2.1 Smallest accepted (SmA) method in ordered model selection

First we recall our setup. Due to the linear structure of the estimators $\tilde{\theta}_m = S_m Y$ and of the loss function $W$, one can consider $\phi_m = \mathcal{K}_m Y$ with $\mathcal{K}_m = WS_m : \mathbb{R}^n \to \mathbb{R}^q$, $m \in \mathbb{M}$, as a family of linear estimators of the $q$-dimensional target of estimation $\phi^* = W\theta^* = WSf^* = \mathcal{K}f^*$ for $\mathcal{K} = W\mathcal{S}$.

Now we discuss a general approach to model selection problems based on multiple testing. Suppose that the given family $\{\phi_m, m \in \mathbb{M}\}$ of estimators is naturally ordered by their complexity (variance). Due to (2.3), this condition can be written as

$$\mathcal{K}_m \text{Var}(\varepsilon) \mathcal{K}_m^\top \leq \mathcal{K}_{m'} \text{Var}(\varepsilon) \mathcal{K}_{m'}^\top, \quad m' > m. \quad (2.4)$$

One would like to pick up a smallest possible index $m \in \mathbb{M}$ which still provides a reasonable fit. The latter means that the bias component

$$\|b_m\|^2 = \|\phi^*_m - \phi^*\|^2 = \|(\mathcal{K}_m - \mathcal{K})f^*\|^2$$
in the risk decomposition (2.3) is not significantly larger than the variance

\[ \text{tr}\{\text{Var}(\tilde{\phi}_m)\} = \text{tr}\{\mathcal{K}_m \text{Var}(\varepsilon)\mathcal{K}_m^\top\}. \]

If \( m^\circ \in \mathcal{M} \) is such a “good” choice, then our ordering assumption yields that a further increase of the index \( m \) over \( m^\circ \) only increases the complexity (variance) of the method without real gain in the quality of approximation. This latter fact can be interpreted in term of pairwise comparison: whatever \( m \in \mathcal{M} \) with \( m > m^\circ \) we take, there is no significant bias reduction in using a larger model \( m \) instead of \( m^\circ \). This leads to a multiple testing procedure: for each pair \( m > m^\circ \) from \( \mathcal{M} \), we consider a hypothesis of no significant bias between the models \( m^\circ \) and \( m \), and let \( \tau_{m,m^\circ} \) be the corresponding test. The model \( m^\circ \) is accepted if \( \tau_{m,m^\circ} = 0 \) for all \( m > m^\circ \). Finally, the selected model is the “smallest accepted”:

\[ \hat{m} \overset{\text{def}}{=} \arg\min\{m^\circ \in \mathcal{M} : \tau_{m,m^\circ} = 0, \forall m > m^\circ\}. \]

Usually the test \( \tau_{m,m^\circ} \) can be written in the form

\[ \tau_{m,m^\circ} = \mathbb{I}\{T_{m,m^\circ} > z_{m,m^\circ}\} \]

for some test statistics \( T_{m,m^\circ} \) and for critical values \( z_{m,m^\circ} \). The information-based criteria like AIC or BIC use the likelihood ratio test statistics

\[ T_{m,m^\circ} = \sigma^{-2}\|\Psi^\top(\tilde{\theta}_m - \tilde{\theta}_{m^\circ})\|^2. \]

A great advantage of such tests is that the test statistic \( T_{m,m^\circ} \) is pivotal \( (\chi^2 \text{ with } m - m^\circ \text{ degrees of freedom}) \) under the correct null hypothesis, this makes it simple to compute the corresponding critical values. Below we apply another choice corresponding to Lepski-type procedure and based on the norm of differences \( \bar{\phi}_m - \bar{\phi}_{m^\circ} :\)

\[ T_{m,m^\circ} = \|\bar{\phi}_m - \bar{\phi}_{m^\circ}\| = \|\mathcal{K}_{m,m^\circ} Y\|, \quad \mathcal{K}_{m,m^\circ} \overset{\text{def}}{=} \mathcal{K}_m - \mathcal{K}_{m^\circ}. \]

The main issue for such a method is a proper choice of the critical values \( z_{m,m^\circ} \). One can say that the procedure is specified by a way of selecting these critical values. Below we offer a novel way of carrying out this choice in a general situation by using a so-called propagation condition: if a model \( m^\circ \) is “good” it has to be accepted with a high probability. This rule can be seen as an analog of the family-wise level condition in a multiple testing problem. Rejecting a “good” model is the family-wise error of first kind, and this error has to be controlled.
2.2 Oracle choice

To specify precisely the meaning of a good model, we use below for each pair $m > m^\circ$ from $M$ the decomposition

$$T_{m,m^\circ} = \|\tilde{\phi}_m - \tilde{\phi}_{m^\circ}\| = \|\mathcal{K}_{m,m^\circ} Y\| = \|\mathcal{K}_{m,m^\circ}(f^* + \varepsilon)\| = \|b_{m,m^\circ} + \xi_{m,m^\circ}\|,$$  \hspace{1cm} (2.5)

where with $\mathcal{K}_{m,m^\circ} = \mathcal{K}_m - \mathcal{K}_{m^\circ}$

$$b_{m,m^\circ} \defeq \mathcal{K}_{m,m^\circ} f^*, \quad \xi_{m,m^\circ} \defeq \mathcal{K}_{m,m^\circ} \varepsilon.$$

We also define

$$b_m \defeq \mathcal{K}_m f^*, \quad \xi_m \defeq \mathcal{K}_m \varepsilon.$$

It obviously holds $IE\xi_{m,m^\circ} = 0$. Introduce the $q \times q$-matrix $\mathbb{V}_{m,m^\circ}$ as the variance of $\tilde{\phi}_m - \tilde{\phi}_{m^\circ}$:

$$\mathbb{V}_{m,m^\circ} \defeq \text{Var}(\tilde{\phi}_m - \tilde{\phi}_{m^\circ}) = \text{Var}(\mathcal{K}_{m,m^\circ} Y) = \mathcal{K}_{m,m^\circ} \text{Var}(\varepsilon) \mathcal{K}_{m,m^\circ}^\top.$$

If the noise $\varepsilon$ is homogeneous with $\text{Var}(\varepsilon) = \sigma^2 I_n$, it holds

$$\mathbb{V}_{m,m^\circ} = \sigma^2 \mathcal{K}_{m,m^\circ} \mathcal{K}_{m,m^\circ}^\top.$$

Further,

$$IE T_{m,m^\circ}^2 = \|b_{m,m^\circ}\|^2 + IE\|\xi_{m,m^\circ}\|^2 = \|b_{m,m^\circ}\|^2 + \mathbb{P}_{m,m^\circ}, \hspace{1cm} (2.6)$$

$$\mathbb{P}_{m,m^\circ} \defeq \text{tr}(\mathbb{V}_{m,m^\circ}) = IE\|\xi_{m,m^\circ}\|^2.$$

The bias term $b_{m,m^\circ} \defeq \mathcal{K}_{m,m^\circ} f^*$ is significant if its squared norm is competitive with the variance term $\mathbb{P}_{m,m^\circ} = \text{tr}(\mathbb{V}_{m,m^\circ})$. We say that $m^\circ$ is a “good” choice if there is no significant bias $b_{m,m^\circ}$ for any $m > m^\circ$. This condition can be quantified in the following “bias-variance trade-off”:

$$\|b_{m,m^\circ}\|^2 \leq \beta^2 \mathbb{P}_{m,m^\circ}, \quad m > m^\circ$$  \hspace{1cm} (2.7)

for a given parameter $\beta$ which controls the bias component in the risk due to decomposition (2.6). Now define the oracle $m^*$ as the minimal $m^\circ$ with the property (2.7):

$$m^* \defeq \min\{m^\circ : \max_{m > m^\circ} \{\|b_{m,m^\circ}\|^2 - \beta^2 \mathbb{P}_{m,m^\circ}\} \leq 0\}.$$

(2.8)
2.3 Tail function, multiplicity correction, critical values $z_{m,m^\circ}$

Now we explain a possible choice of critical values $z_{m,m^\circ}$ in the situation when the noise distribution is known. A particular example is the case of Gaussian errors $\varepsilon \sim \mathcal{N}(0,\sigma^2 I_n)$. Then the distribution of the stochastic component $\xi_{m,m^\circ}$ is known as well. In the Gaussian case, it is $\mathcal{N}(0,V_{m,m^\circ})$ with the covariance matrix $V_{m,m^\circ}$. Introduce for each pair $m > m^\circ$ from $M$ a tail function $z_{m,m^\circ}(t)$ of the argument $t$ such that

$$\mathbb{P}\left(\|\xi_{m,m^\circ}\| > z_{m,m^\circ}(t)\right) = e^{-t}. \quad (2.9)$$

Here we assume that the distribution of $\|\xi_{m,m^\circ}\|$ is continuous and the value $z_{m,m^\circ}(t)$ is well defined. Otherwise one has to define $z_{m,m^\circ}(t)$ as the smallest value for which the error probability is smaller than $e^{-t}$.

For checking the propagation condition, we need a uniform in $m > m^\circ$ version of the probability bound (2.9). Let

$$M^+(m^\circ) \overset{\text{def}}{=} \{m \in M : m > m^\circ\}. \quad (2.10)$$

Given $x$, by $q_{m^\circ} = q_{m^\circ}(x)$ denote the corresponding multiplicity correction:

$$\mathbb{P}\left(\bigcup_{m \in M^+(m^\circ)} \{\|\xi_{m,m^\circ}\| \geq z_{m,m^\circ}(x + q_{m^\circ})\}\right) = e^{-x}. \quad (2.10)$$

A simple way of computing the multiplicity correction $q_{m^\circ}$ is based on the Bonferroni bound: $q_{m^\circ} = \log(\#M^+(m^\circ))$. However, it is well known that the Bonferroni bound is very conservative and leads to a large correction $q_{m^\circ}$, especially if the random vectors $\xi_{m,m^\circ}$ are strongly correlated. This is exactly the case under consideration. Note that the joint distribution of the $\xi_{m,m^\circ}$’s is precisely known. This allows to define the correction $q_{m^\circ} = q_{m^\circ}(x)$ just by condition (2.10). Finally we define the critical values $z_{m,m^\circ}$ by one more correction for the bias:

$$z_{m,m^\circ} \overset{\text{def}}{=} z_{m,m^\circ}(x + q_{m^\circ}) + \beta \sqrt{p_{m,m^\circ}} \quad (2.11)$$

for $p_{m,m^\circ} = \text{tr}(V_{m,m^\circ})$. This definition still involves two numerical tuning constants $x$ and $\beta$. The first value $x$ controls the nominal rejection probability under the null, a usual choice $x = 3$ does a good job in most of cases. The value $\beta$ controls the amount of admissible bias in the definition of a good choice; cf. (2.7) and (2.8). This value is mainly for theoretical study, in practice one can always take $\beta = 0$. 

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2.4 SmA choice and the oracle inequality

Define the selector \( \hat{m} \) by the “smallest accepted” (SmA) rule. Namely, with \( \hat{m}_{m, m^\circ} \) from (2.11), the acceptance rule reads as follows:

\[
\{ \text{\( m^\circ \) is accepted} \} \Leftrightarrow \left\{ \max_{m \in M^+ (m^\circ)} \{ T_{m, m^\circ} - \hat{m}_{m, m^\circ} \} \leq 0 \right\}.
\]

The SmA rule is

\[
\hat{m} \overset{\text{def}}{=} \text{“smallest accepted”} = \min \left\{ m^\circ : \max_{m \in M^+ (m^\circ)} \{ T_{m, m^\circ} - \hat{m}_{m, m^\circ} \} \leq 0 \right\}.
\]

(2.12)

Our study mainly focuses on the behavior of the selector \( \hat{m} \). The performance of the resulting estimator \( \hat{\phi} = \hat{\phi}_{\hat{m}} \) is a kind of corollary from statements about the selected model \( \hat{m} \). The ideal solution would be \( \hat{m} \equiv m^* \), then the adaptive estimator \( \hat{\phi} \) coincides with the oracle estimate \( \tilde{\phi}_{m^*} \).

The bound (2.9) automatically ensures the desired propagation property: any good model \( m^\circ \) in the sense (2.7) will be accepted with probability at least \( 1 - e^{-x} \). In some sense, this property is built-in by the construction of the procedure. By definition, the oracle \( m^* \) is also a “good” choice, this yields

\[
P(\text{\( m^* \) is rejected}) \leq e^{-x}.
\]

(2.13)

Therefore, the selector \( \hat{m} \) typically takes its value in \( M^-(m^*) \), where

\[
M^-(m^*) = \{ m \in M : m < m^* \}
\]

is the set of all models in \( M \) smaller than \( m^* \). It remains to check the performance of the method in this region. The next step is to specify a subset \( M^0 \) of \( M^-(m^*) \) of highly probable \( \hat{m} \)-values. We will refer to this subset as the zone of insensitivity. The definition of \( m^* \) implies that there is a significant bias for each \( m \in M^-(m^*) \). If this bias is really large, then, again, the probability of selecting \( m \) can be bounded from above by a small value. Therefore, the zone of insensitivity is composed of \( m \)-values for which the bias is significant but not very large.

Now we present a formal description which specifies a subset \( M^c \) of \( M^-(m^*) \) for which the bias \( \|b_{m^*, m}\| \) is sufficiently large and hence, the probability of the event \( \{ \hat{m} \in M^c \} \) is negligible.

**Theorem 2.1.** Let \( z_{m, m^\circ} (\cdot) \) be the tail function from (2.9) for each pair \( m > m^\circ \in M \). Given \( x \) and \( \beta \), let \( \hat{m}_{m, m^\circ} \) be given by (2.10) and (2.11). Then the propagation property
(2.13) is fulfilled for the SmA selector $\hat{m}$. Moreover, for any subset $M^c \subseteq M^{-}(m^*)$ s.t.
\[
\|b_{m^*,m}\| > \bar{z}_{m^*,m} + z_{m^*,m}(x_s), \quad m \in M^c,
\] (2.14)
for $x_s \equiv x + \log(|\mathcal{M}^c|)$ with $|\mathcal{M}^c|$ being the cardinality of $M^c$, it holds
\[
\mathcal{P}(\hat{m} \in M^c) \leq e^{-x}.
\]
The SmA estimator $\hat{\phi} = \tilde{\phi}_{\hat{m}}$ satisfies the following bound:
\[
\mathcal{P}(\|\hat{\phi} - \tilde{\phi}_{m^*}\| > \bar{\tilde{z}}_{m^*}) \leq 2e^{-x},
\] (2.15)
where $\bar{\tilde{z}}_{m^*}$ is defined with $\mathcal{M}^o \equiv \mathcal{M}^{-}(m^*) \setminus M^c$ as
\[
\bar{\tilde{z}}_{m^*} \equiv \max_{m \in \mathcal{M}^o} \bar{z}_{m^*,m}.
\] (2.16)
This implies the probabilistic oracle bound: with probability at least $1 - 2e^{-x}$
\[
\|\hat{\phi} - \phi^*\| \leq \|\tilde{\phi}_{m^*} - \phi^*\| + \bar{\tilde{z}}_{m^*}.
\] (2.17)

Remark 2.1. Note that the choice $x_s = x + \log(|\mathcal{M}^c|)$ relies on crude Bonferroni arguments and the definition of $M^c$ can be refined by choosing $x_s$ more carefully. However, this value only enters in the theoretical bound and is not used in the procedure, a fine tuning for this value is not required. Obviously $x_s \leq x + \log(|\mathcal{M}^{-}(m^*)|)$.

Remark 2.2. The result (2.17) is called the oracle bound because it compares the loss of the data-driven selector $\hat{m}$ and of the optimal choice $m^*$. The value $\bar{\tilde{z}}_{m^*}$ in (2.16) can be viewed as a “payment for adaptation”. An interesting feature of the presented result is that not only the oracle quality but also the payment for adaptation depend upon the unknown response $f^*$ and the corresponding oracle choice $m^*$. In the worst case of a model with a flat risk profile $R_m$, the set $\mathcal{M}^o$ can coincide with the whole range $\mathcal{M}^{-}(m^*)$. Even in this case the bounds (2.15) and (2.17) are meaningful. However, the payment for adaptation $\bar{\tilde{z}}_{m^*}$ in this case can be larger than the oracle risk. In the contrary, if the risk function $R_m$ grows rapidly as $m$ decreases below $m^*$, then the set $\mathcal{M}^o$ is small and the value $\bar{\tilde{z}}_{m^*}$ is much smaller than the oracle risk $R_{m^*}$.

2.5 Analysis of the payment for adaptation $\bar{\tilde{z}}_{m^*}$

Here we present an upper bound on $\bar{\tilde{z}}_{m^*}$ for a special case of Gaussian independent errors $\varepsilon_i$. The benefit of considering the Gaussian case is that each vector $\xi_{m',m}$ is Gaussian as well, which simplifies the analysis of the tail function $z_{m',m}(\cdot)$. However, the results
can be extended to non-Gaussian errors $\varepsilon_i$ under exponential moment conditions. Below $m_0$ denotes the smallest model in $M$. Writing $V_m \triangleq \sigma^2 K_m K_m^\top$, we define

$$p_m \triangleq \text{tr}(V_m)$$

$$\lambda_m \triangleq \|V_m\|_{\text{op}}.$$

**Theorem 2.2.** Assume the conditions of Theorem 2.1. Let also $p_{m,m^*} = \text{tr}(V_{m,m^*})$ and $\lambda_{m,m^*} = \|V_{m,m^*}\|_{\text{op}}$ with $V_{m,m^*} = \text{Var}(\xi_{m,m^*})$ satisfy $p_{m^*,m} \leq p_{m^*,m_0} \leq p_{m^*}$ and $\lambda_{m^*,m} \leq \lambda_{m^*,m_0} \leq \lambda_{m^*}$ for all $m_0 \leq m < m^*$. If the errors $\varepsilon_i$ are normal zero mean then the critical values $\gamma_{m,m^*}$ given by (2.11) satisfy

$$\gamma_{m,m^*} \leq (1 + \beta) \sqrt{p_{m,m^*}} + \sqrt{2 \lambda_{m,m^*} \{x + \log(|M|)\}},$$

while the payment for adaptation $\zeta_{m^*}$ follows the bound

$$\zeta_{m^*} \leq (1 + \beta) \sqrt{p_{m^*}} + \sqrt{2 \lambda_{m^*} \{x + \log(|M|)\}} \leq (1 + \beta) \sqrt{p_{m^*}} + \sqrt{2 \lambda_{m^*} \{x + \log(|M|)\}}.$$

Some special cases of this result for projection and linear functional estimation will be discussed in Sections 2.7 and 2.8 below.

### 2.6 Power loss function

The probabilistic oracle bound of Theorem 2.1 provides some statement about typical behavior of the adaptive SmA estimate $\hat{\phi} = \tilde{\phi}_m$. Unfortunately, this bound does not yield a risk bound for quadratic or polynomial losses: even if big losses occur with a small probability, the related risk can still be large. It happens that the SmA procedure can be easily tuned to secure an oracle risk bound.

For simplicity of notation, we only consider the quadratic risk

$$\mathcal{R}(\hat{\phi}) \triangleq E\|\hat{\phi} - \phi^*\|^2.$$

We aim at comparing the risk of the SmA procedure with the risk $\mathcal{R}_{m^*}$ of the oracle estimate $\tilde{\phi}_{m^*}$. Recall the representation

$$\mathcal{R}_m \triangleq E\|\tilde{\phi}_m - \phi^*\|^2 = E\|\xi_m\|^2 + \|b_m\|^2 = p_m + \|b_m\|^2$$

with $p_m = \text{tr}(V_m)$ and $V_m = \text{Var}(\xi_m)$. For our analysis, we have to slightly modify the definition of the oracle (2.8). Namely, to ensure an oracle risk bound, we require that
not only the model \( m^* \) is “good” but also all the larger models \( m > m^* \) are “good” as well:

\[
m^* \equiv \min \left\{ m^0 : \max_{m', m \in M^+(m^0) : m' > m} \left\{ \| b_{m', m} \|^2 - \beta^2 p_{m', m} \right\} \leq 0 \right\}.
\]

(2.18)

Below we also suppose that the bias component \( \| b_m \|^2 \) fulfills

\[
\| b_m \| \leq \| b_{m^*} \|, \quad m > m^*.
\]

(2.19)

Otherwise, one can define \( \| b_{m^*} \| \equiv \max_{m \in M^+(m^*)} \| b_m \| \).

The choice of the critical values \( z_{m', m} \) for the SmA procedure has to be slightly changed to ensure a risk bound for quadratic loss. For this, we need a bit more detailed analysis of the SmA procedure in the propagation zone \( m > m^* \). In this zone the variance dominates the bias, therefore, the SmA procedure can be tuned in the situation when there is no signal and hence no bias at all:

\[
T_{m', m} = \| \phi_{m'} - \phi_m \| = \| \xi_{m', m} \|.
\]

The analysis is based on a simple but important observation that if \( \hat{m} = m > m^* \), then the good model \( m^0 = m_{[-1]} \) is rejected, where \( m_{[-1]} \) denotes the next smaller model with respect to \( m \). The latter means that at least one check based on \( T_{m', m_{[-1]}} \) fails. The same can be expressed as follows: the maximum of the r.v.’s \( T_{m', m_{[-1]}} I(T_{m', m_{[-1]}} > z_{m', m_{[-1]}}) \) is positive. For a formal description, introduce for each \( m \) and \( x \) a random event

\[
A_m(x) \equiv I\left( \max_{m' \in M^+(m)} \{ \| \xi_{m', m} \| - z_{m', m(x)} \} > 0 \right)
\]

on which at least one of the test statistics \( T_{m', m} = \| \xi_{m', m} \| \) exceeds the critical value \( z_{m', m(x)} \). The case of probabilistic loss focuses on the probability of this event, the value \( x \) is selected to make it small enough. Now, under the polynomial loss function, we need a bound for the moment of the corresponding loss. Namely, for each \( m \), consider the expectation of \( p_m^{-1} \| \xi_m \|^2 \) on the random set \( A_{m(-1)}(x) \):

\[
R_m^+(x) \equiv E \left[ (p_m^{-1} \| \xi_m \|^2 \vee 1) I\left( \max_{m' \in M^+(m_{[-1]}, m \in M^+(m_{[-1]}))} \{ \| \xi_{m', m_{[-1]}}, m \| - z_{m', m_{[-1]}}(x) \} > 0 \right) \right].
\]

Similarly one can consider any other power loss function by replacing \( (p_m^{-1/2} \| \xi_m \|)^2 \) with \( (p_m^{-1/2} \| \xi_m \|)^q \). In particular, \( q = 0 \) yields the probability loss considered before.

Now we define the value \( x_{m_{[-1]}} \) in such a way that the related deviation risk \( R_m^+(x) \) can be controlled from above. Let \( \alpha_m \) be a given decreasing sequence. Its choice will be
discussed below. We fix for each \( m \) the value \( x_{m_{(1)}} \) such that

\[
\mathcal{R}_m^+(x_{m_{(1)}}) = \alpha_m. \tag{2.20}
\]

It implies

\[
IE\left[\|\xi_m\|^2 \mathbb{I}\left(A_{m_{(1)}}(\mathbf{x})\right)\right] \leq \alpha_m p_m, \tag{2.21}
\]

\[
\mathbb{P}\left(A_{m_{(1)}}(\mathbf{x})\right) \leq \alpha_m.
\]

Now define the critical values \( \bar{z}_{m,m^\circ} \) of the SmA procedure as

\[
\bar{z}_{m,m^\circ} = z_{m,m^\circ}(x_{m^\circ}) + \beta p_{m,m^\circ}^{1/2}. \tag{2.22}
\]

The resulting procedure reads exactly as in the case of probabilistic loss:

\[
\hat{m} = \min\left\{ m^\circ: \max\{T_{m,m^\circ} - \bar{z}_{m,m^\circ} \leq 0\} \right\}. \tag{2.23}
\]

It is worth mentioning that the procedure is the same, and even the critical values \( \bar{z}_{m,m^\circ} \) are given by the same formula, as in the case of probabilistic loss. The only difference is in the propagation condition (2.20) which is a bit stronger than a similar condition for indicator loss. This implies that the values \( x_{m^\circ} \) and \( \bar{z}_{m,m^\circ} \) are a bit larger in the case of a power loss function.

**Theorem 2.3.** Let the SmA procedure (2.23) be applied with the critical values \( \bar{z}_{m,m^\circ} \) from (2.22), where the values \( x_m \) are defined by (2.20) with the coefficients \( \alpha_m \) satisfying

\[
\sum_{m \in \mathcal{M}^+(m^\circ)} \alpha_m p_m \leq \bar{\alpha}_{m^\circ} p_{m^\circ} \tag{2.24}
\]

for some \( \bar{\alpha}_{m^\circ} \). If the errors \( \varepsilon_i \) are normal zero mean, then

\[
IE\left[\|\hat{\phi} - \phi^*\|^2 \right] \leq 2\bar{\alpha}_{m^\circ} R_{m^\circ} + \left(\mathcal{R}_{m^\circ}^{1/2} + \bar{z}_{m^\circ} \right)^2, \tag{2.25}
\]

where

\[
\bar{z}_{m^\circ} \overset{\text{def}}{=} \max_{m \in \mathcal{M}^-(m^\circ)} \bar{z}_{m,m^\circ}.
\]

Similarly to the probabilistic loss function, the result can be refined by considering the zone of insensitivity in the region \( m < m^\circ \).

Now we briefly discuss the choice of constants \( \alpha_m \) entering into (2.24). Suppose that the \( p_m \)'s satisfy

\[
\sum_{m \in \mathcal{M}^+(m^\circ)} (p_{m^\circ}/p_m)^a \leq C \tag{2.26}
\]
for some \( a > 0 \) and a fixed constant \( C \). Then one can take
\[
\alpha_m = \left( \frac{p_m}{p_{m_0}} \right)^{1-a}.
\]

Below we focus on a situation when the effective dimension \( p_m \) grows exponentially with \( m \). Note that this situation is typical in model selection and often one can reduce the general case to this one by a proper discretization. Then (2.26) is fulfilled for any \( a > 0 \) with \( C = C(a) \).

The further step is an upper bound on the values \( x_m, z_{m,m^o}(x_m) \), and \( \delta_{m,m^o} \), as well as on the payment for adaptation \( \delta_{m^*} \). These bounds require some exponential moment conditions on the errors \( \varepsilon_i \). To reduce the computational burden, we again focus on the case of Gaussian errors.

**Proposition 2.4.** Suppose (2.26) for \( a > 0 \). If the errors \( \varepsilon_i \) are normal zero mean, then the choice
\[
\alpha_m = \sqrt{3} \left( \frac{p_m}{p_{m_0}} \right)^{1-a}, \quad x_{m(-1)} = 2(1 + a) \log \left( \frac{p_m}{p_{m_0}} \right),
\]
ensures conditions (2.24), (2.20), and therefore, the oracle bound (2.25) with \( \pi_{m^*} = \sqrt{3}C \left( \frac{p_{m_0}}{p_{m^*}} \right)^{1+a} \). Furthermore,
\[
\delta_{m^*} \leq \beta \sqrt{p_{m^*}} + \sqrt{2}\lambda_{m^*} \{ 2(1 + a) \log \left( \frac{p_{m^*}}{p_{m_0}} \right) + \log (\|M\|) \}.
\]

2.7 **Application to projection estimation**

An important feature of the obtained oracle statements is their universality: they equally apply to various setups and problems and provide some quantitative explicit error bounds even for finite samples. Below we briefly comment on two popular cases of projection estimation and estimation of a linear functional. In some sense, these are two extreme cases of relation between \( p_{m^*} \) and \( \lambda_{m^*} \).

This section discusses the case of projection estimation in the linear model \( Y = \Psi^\top \theta^* + \varepsilon \) with homogeneous errors \( \varepsilon_i \): \( \text{Var}(\varepsilon_i) = \sigma^2 \). All the conclusions can be easily extended to heterogeneous errors whose variances are contained in some fixed interval. We also focus on probabilistic loss, the case of polynomial loss can be considered in the same way.

Let us assume an ordering on the features of \( \Psi_m \) and let for each \( m \in \mathbb{N} \) denote \( \Psi_m \) as the submatrix \( \Psi \) corresponding to first \( m \) features, i.e. the projector onto the first \( m \) features. We use \( m \) to denote the model and the number of features. The related estimator \( \hat{\theta}_m \) is the standard LSE with \( S_m = (\Psi_m \Psi_m^\top)^{-1} \Psi_m \) and the prediction problem with \( W = \Psi^\top \) yields \( \mathcal{K}_m Y = \Pi_m Y \) where \( \Pi_m = \Psi_m^\top (\Psi_m \Psi_m^\top)^{-1} \Psi_m \) is the projector.
onto the corresponding feature subspace. For homogeneous errors $\varepsilon_i$ with $\text{Var}(\varepsilon_i) = \sigma^2$, the variance $\mathbb{V}_m = \text{Var}(\Pi_m \mathbf{Y})$ satisfies

$$p_m = \text{tr}\{\text{Var}(\Pi_m \mathbf{Y})\} = \sigma^2 \text{tr}(\Pi_m) = \sigma^2 m.$$ 

Moreover, for each pair $m > m^\circ$, it holds

$$\Psi^\top (\tilde{\theta}_m - \tilde{\theta}_{m^\circ}) = (\Pi_m - \Pi_{m^\circ}) \mathbf{Y} = \Pi_{m,m^\circ} \mathbf{Y},$$

where $\Pi_{m,m^\circ}$ projects on the subspace of features entering in $m$ but not in $m^\circ$.

**Corollary 2.5.** Consider the problem of projection estimation with homogeneous Gaussian errors $\varepsilon_i$ and probabilistic loss. Then $p_{m,m^\circ} = \sigma^2 (m - m^\circ)$, $\lambda_{m,m^\circ} = \sigma^2$, and

$$\mathbb{Z}_{m,m^\circ} \leq \sigma (1 + \beta) \sqrt{m - m^\circ} + \sigma \sqrt{2x + 2 \log(|\mathcal{M}|)},$$

$$\mathbb{Z}_{m^*} \leq \sigma (1 + \beta) \sqrt{m^*} + \sigma \sqrt{2x + 2 \log(|\mathcal{M}|)}.$$ 

The first term in the expression for $\mathbb{Z}_{m^*}$ is of order $\sqrt{m^*}$ and it is a leading one provided that the effective dimension $m^*$ is essentially larger than $\log(|\mathcal{M}|)$. Usually the cardinality of the set $\mathcal{M}$ is only logarithmic in the sample size $n$; cf. Lepski (1991); Lepski et al. (1997). Then $\log(|\mathcal{M}|) \approx \log \log n$ and $\mathbb{Z}_{m^*} \approx \sigma \sqrt{m^*}$ for $m^* \gg \log \log n$.

For the oracle risk $R_{m^*}$, it holds $R_{m^*} = p_{m^*} + \|b_{m^*}\|^2 \geq \sigma^2 m^*$. Therefore, the payment for adaptation $\mathbb{Z}_{m^*}$ is of the same order as the square root of the oracle risk, and the result of Proposition 2.2 has a surprising corollary: rate adaptive estimation is possible if the oracle dimension $m^*$ is significantly larger than $\log \log n$.

**Remark 2.3.** The payment for adaptation can be drastically reduced in the situations with a narrow zone of insensitivity. If the bias grows rapidly when $m$ decreases from $m^*$ to $m_0$, more precisely, if $\|b_{m^*,m}\|^2 \geq C \sigma^2 (m^* - m + 2x + 2 \log(|\mathcal{M}|))$ for some fixed constant $C$ and all $m \leq m^\circ$ with $m^\circ < m^*$, then

$$\mathbb{Z}_{m^*} \leq \sigma (1 + \beta) \sqrt{m^* - m^\circ} + \sigma \sqrt{2x + 2 \log(|\mathcal{M}|)).}$$

So, if $(m^* - m^\circ)/m^*$ is small, the payment for adaptation is smaller in order than the oracle risk, and the procedure is sharp adaptive. In particular, one can easily see that the self-similarity condition of Gine and Nickl (2010) ensures a rapid growth of the bias when the index $m$ becomes smaller than $m^*$. This in turn yields a narrow zone of insensitivity and hence, a sharp adaptive estimation.

**Remark 2.4.** It is worth mentioning the relation of the proposed procedure to the popular Akaike (AIC) criterion. AIC defines $\hat{m}$ by minimizing

$$\hat{m} = \arg\min_m \{\| \mathbf{Y} - \Pi_m \mathbf{Y} \|^2 + 2 \sigma^2 m\}.$$
One can easily see that this rule is equivalent to the SmA rule (2.12) with $\hat{z}_{m,m^*}^2 = 2\sigma^2(m - m^*)$. However, this choice does not guarantee the propagation condition (2.13).

2.8 Linear functional estimation

In this section, we discuss the problem of linear functional estimation. As previously, we assume a family of estimators $\tilde{\phi}_m = \mathcal{K}_m Y$, $m \in M$, to be given, where the rank of each $\mathcal{K}_m$ is equal to 1. The ordering condition means that these estimators are ordered by their variance:

$$v_m^2 \overset{\text{def}}{=} \text{Var}(\mathcal{K}_m Y) = \mathcal{K}_m \text{Var}(\varepsilon) \mathcal{K}_m^\top$$ \hspace{1cm} (2.29)

grows with $m$. Further, each stochastic component $\xi_{m,m^*} = \mathcal{K}_{m,m^*} \varepsilon$ is one-dimensional, and it holds

$$\lambda_{m,m^*} = p_{m,m^*} = v_{m,m^*}^2 = \mathcal{K}_{m,m^*} \text{Var}(\varepsilon) \mathcal{K}_{m,m^*}^\top.$$

Note that in the case of Gaussian errors, $\xi_{m,m^*}$ is also Gaussian: $\xi_{m,m^*} \sim N(0, v_{m,m^*}^2)$. The tail function $z_{m,m^*}(x)$ of $\xi_{m,m^*}$ can be upper-bounded by $v_{m,m^*} \sqrt{2x}$. In the case of probabilistic loss, a Bonferroni correction and a bias adjustment lead to the upper bound for the critical values $\hat{z}_{m,m^*}$:

$$\hat{z}_{m,m^*} \leq v_{m,m^*} \left( \beta + \sqrt{2x + 2 \log(|M|)} \right),$$ \hspace{1cm} (2.30)

where $|M|$ is the number of elements in $M$. This implies

$$\tilde{z}_{m^*} \leq v_{m^*} \left( \beta + \sqrt{2x + 2 \log(|M|)} \right).$$ \hspace{1cm} (2.31)

**Theorem 2.6.** Let the errors $\varepsilon_i$ be Gaussian zero mean. Consider a problem of linear functional estimation of $\phi^* = \mathcal{K} f^*$ by a given family $\tilde{\phi}_m = \mathcal{K}_m Y$ with $\text{rank}(\mathcal{K}_m) = \text{rank}(\mathcal{K}) = 1$, $m \in M$. Then the critical values $\hat{z}_{m,m^*}$ from (2.11) fulfill (2.30) and the oracle inequality (2.17) holds with the payment for adaptation $\tilde{z}_{m^*}$ obeying (2.31).

**Remark 2.5.** One can conclude that for the problem of functional estimation with probabilistic loss, the squared payment for adaptation $\tilde{z}_{m^*}^2$ is by factor $\log(|M|)$ larger than the oracle variance $v_{m^*}^2$. If $|M|$ itself is logarithmic in the sample size $n$, we end up with the extra $(\log \log n)$-factor in the accuracy of adaptive estimation.

In the case of polynomial loss, similar arguments yield due to (2.22) and (2.27)

$$\hat{z}_{m,m^*} \leq v_{m,m^*} \left( \beta + \sqrt{2x_{m^*} + 2 \log(|M|)} \right) \leq v_{m,m^*} \left( \beta + \sqrt{2(1 + a) \log(p_{m^*}/p_{m_0}) + 2 \log(|M|)} \right)$$
Spokoiny and Vial (2009) showed that the bound $\tilde{j}_{m,m^\circ}^2 \geq C v_{m,m^\circ}^2 (m^\circ - m_0)$ is necessary to ensure a propagation condition for geometrically growing variance $p_m = v_m^2$. The bound (2.30) yields

$$\tilde{j}_{m^*} \leq v_{m^*} \left( \beta + \sqrt{2(1 + a) \log(v_{m^*}^2/v_{m_0}^2)} + 2 \log(|M|) \right).$$

(2.32)

**Theorem 2.7.** Suppose that the errors $\varepsilon_i$ are Gaussian zero mean. Let the family of functional estimators $\mathcal{K}_m Y$ be such that the variances $p_m = v_m^2$ from (2.29) fulfill the condition (2.26) with $a > 0$. Then the critical values $\tilde{j}_{m,m^\circ}$ from (2.22) for the SmA procedure fulfill (2.30). For the resulting selector $\hat{m}^*$, the oracle inequality (2.25) holds and the payment for adaptation $\tilde{j}_{m^*}$ follows (2.32).

**Remark 2.6.** It appears that polynomial loss yields a larger price for adaptation: $\tilde{j}_{m^*}^2 \times v_{m^*}^2 \log(v_{m^*}^2/v_{m_0}^2)$. This conclusion is consistent with the results by Lepski (1992) and Cai and Low (2003, 2005) which show that the log-price for adaptation cannot be avoided if a polynomial loss function is considered. Our result seems to be even more informative because it delivers a non-asymptotic error bound which adapts to the underlying unknown model.

### 3 Bootstrap tuning

This section explains how the proposed SmA procedure can be applied if no information about the noise $\varepsilon = Y - \mathbb{E}Y$ is available.

#### 3.1 Presmoothing and wild bootstrap

Let the observed data $Y$ follow the model $Y = f^* + \varepsilon$ with $\varepsilon \sim \mathcal{N}(0, \Sigma)$, where $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_n^2)$ is an unknown diagonal covariance matrix. We assume that the response vector $f^*$ can be well approximated by a linear expansion for a given basis $\Psi$ in the form $f^* \approx \Psi^\top \theta^*$. The vector $\theta^*$ can be naturally treated as target of estimation. Assume we are given the ordered family of the estimators $(\tilde{\theta}_m)$ of $\theta^*$:

$$\tilde{\theta}_m = \mathcal{S}_m Y = (\Psi_m \Psi_m^\top)^{-1} \Psi_m Y, \quad m \in M.$$  

For each pair $m > m^\circ$ from $M$, we consider the test statistic $T_{m,m^\circ}$ and its decomposition from (2.5): with $\mathcal{K}_{m,m^\circ} = W(\mathcal{S}_m - \mathcal{S}_{m^\circ})$

$$T_{m,m^\circ} = \|\mathcal{K}_{m,m^\circ} Y\| = \|\mathcal{K}_{m,m^\circ}(f^* + \varepsilon)\| = \|b_{m,m^\circ} + \xi_{m,m^\circ}\|,$$

Calibration of the SmA model selection procedure requires to know the joint distribution of all corresponding stochastic terms $\|\xi_{m,m^\circ}\|$ for $m > m^\circ$ which is uniquely determined.
by the noise covariance matrix $\Sigma$. In the case when this matrix is unknown, we are going to use a bootstrapping procedure to approximate this distribution.

The proposed procedure relates to the concept of the wild bootstrap, Wu (1986), Beran (1986). In the framework of a regression problem, it suggests to model the unknown heteroscedastic noise using randomly weighted residuals from pilot estimation. We apply normal weights. For other possible bootstrap weights see for example Mammen (1993).

Suppose we are given a pilot estimator (presmoothing) $\tilde{f}$ of the response vector $f^* \in \mathbb{R}^n$. Define the residuals:

$$\tilde{Y} \overset{\text{def}}{=} Y - \tilde{f}.$$ 

This pilot is supposed to undersmooth, that is, the bias is negligible and the variance of $\tilde{Y}$ is close to $\Sigma$. This pre-smoothing requires some minimal smoothness of the regression function, and this condition seems to be unavoidable if no information about the noise is given: otherwise one cannot distinguish between signal and noise. Below we suppose that $\tilde{f}$ is a linear predictor, $\tilde{f} = \Pi Y$, where $\Pi$ is a sub-projector in the space $\mathbb{R}^n$. For example, one can take $\Pi = \psi_{m^\dagger}^T (\psi_{m^\dagger}^T \psi_{m^\dagger})^{-1} \psi_{m^\dagger}$ where $m^\dagger$ is a large model, e.g. the largest model $M$ in our collection.

The wild bootstrap proposes to resample from the heteroscedastic Gaussian noise $I\bar{P}^\flat = N(0, \tilde{\Sigma})$ with

$$\tilde{\Sigma} = \text{diag}(\tilde{Y} \cdot \tilde{Y}),$$

where $\tilde{Y} \cdot \tilde{Y}$ denotes the coordinate-wise product of the vector $\tilde{Y}$ with itself and $\text{diag}(\tilde{Y} \cdot \tilde{Y})$ denotes the diagonal matrix with entries from $\tilde{Y} \cdot \tilde{Y}$. These entries depend on $Y$ and thus are random. Therefore, the bootstrap distribution $I\bar{P}^\flat$ is a random measure on $\mathbb{R}^n$ and the aim of our study is to show that this random measure mimics well the underlying data distribution for typical realizations of $Y$. Clearly $\text{diag}(\tilde{Y} \cdot \tilde{Y})$ is a very bad estimator of the covariance matrix $\Sigma$. However, below we show that under realistic conditions on the pilot $\tilde{f}$ and on the model, it does a good job and allows to obtain essentially the same results as in the case of known $\Sigma$.

Let $w^\flat$ denote the $n$-vector of bootstrap weights $w^\flat \sim N(0, I_n)$. Clearly the product $\varepsilon^\flat = \text{diag}(\tilde{Y}) w^\flat$ is conditionally on $Y$ normal,

$$\varepsilon^\flat = \text{diag}(\tilde{Y}) w^\flat \mid Y \sim N(0, \tilde{\Sigma}).$$

Bootstrap analog of $\xi_{m,m^\circ} = K_{m,m^\circ} \varepsilon$ reads $\xi_{m,m^\circ}^\flat = K_{m,m^\circ} \varepsilon^\flat = K_{m,m^\circ} \text{diag}(\tilde{Y}) w^\flat$ and

$$\|\xi_{m,m^\circ}^\flat\| \overset{\text{def}}{=} \|K_{m,m^\circ} \text{diag}(\tilde{Y}) w^\flat\|.$$ (3.1)
The idea is to calibrate the SmA procedure under the bootstrap measure \( P^b \) using \( \| \xi_{m,m^o}^b \| \) in place of \( \| \xi_{m,m^o} \| \). The bootstrap quantiles \( z_{m,m^o}^b(t) \) are given by analog of (2.9):

\[
P^b\left( \| \xi_{m,m^o}^b \| > z_{m,m^o}^b(t) \right) = e^{-t}.
\] (3.2)

The multiplicity correction \( q_{m^o}^b = q_{m^o}^b(x) \) is specified by the condition

\[
P^b\left( \bigcup_{m \in M^+(m^o)} \{ \| \xi_{m,m^o}^b \| \geq z_{m,m^o}^b(x + q_{m^o}^b) \} \right) = e^{-x}.
\] (3.3)

Finally, the bootstrap critical values are fixed by the analog of (2.11):

\[
\tilde{z}_{m,m^o}^b \overset{def}{=} z_{m,m^o}^b(x + q_{m^o}^b) + \beta \sqrt{p_{m,m^o}^b}
\]

for \( p_{m,m^o}^b = E^b\| \xi_{m,m^o}^b \|^2 \) given by

\[
p_{m^o,m}^b \overset{def}{=} \text{tr}(K_{m^o,m} \text{diag} \left( \tilde{Y} \right) K_{m^o,m}).
\]

Recall that all these quantities are data-driven and depend upon the original data. Now we apply the SmA procedure with the critical values \( \tilde{z}_{m,m^o}^b \) defined in such a way. Our main result claims that this choice still ensures the propagation condition (2.10) and therefore, all the obtained results including the oracle bounds, apply for this choice as well; see Theorem 3.2. Moreover, we evaluate the distance between the unknown underlying data distribution \( P \) and the bootstrap distribution \( P^b \). The latter is random, however, we show that with high probability, it is close to its deterministic counterpart \( P \). To make the results transparent and concise we assume a heterogeneous Gaussian noise \( \varepsilon \). All the statements can be extended to a non-Gaussian noise under some exponential moment conditions at the cost of many technical details.

Let \( Q \) denote the joint distribution of all stochastic vectors \( \xi_{m,m^o} \) entering in the decomposition of the test statistics \( T_{m,m^o} \) for \( m > m^o \). Let also \( Q^b \) be the similar distribution of the bootstrapized stochastic vectors \( \xi_{m,m^o}^b \) entering in the test statistics \( T_{m,m^o}^b \). The next result allows to upper bound the total variation distance between \( Q \) and \( Q^b \) in terms of the following quantities:

**Design Regularity** is measured by the value \( \delta_{\psi} \)

\[
\delta_{\psi} \overset{def}{=} \max_{i=1,\ldots,n} \| S^{-1/2} \psi_i \| \sigma_i, \quad \text{where} \quad S \overset{def}{=} \sum_{i=1}^n \psi_i \psi_i^\top \sigma_i^2;
\] (3.4)

Obviously

\[
\sum_{i=1}^n \| S^{-1/2} \psi_i \|^2 \sigma_i^2 = \text{tr} \left( \sum_{i=1}^n S^{-2} \psi_i \psi_i^\top \sigma_i^2 \right) = \text{tr} I_p = p,
\]
and therefore in typical situations the value $\delta_\psi$ is of order $\sqrt{p/n}$.

**Presmoothing bias** for a projector $\Pi$ is described by the vector

$$B = \Sigma^{-1/2}(f^* - \Pi f^*).$$

(3.5)

We will use the sup-norm $\|B\|_\infty = \max_i |b_i|$ and the squared $\ell_2$-norm $\|B\|^2 = \sum_i b_i^2$ to measure the bias after presmoothing.

**Stochastic noise after presmoothing** is described via the covariance matrix $\text{Var}(\tilde{\varepsilon})$ of the smoothed noise $\tilde{\varepsilon} = \Sigma^{-1/2}(\varepsilon - \Pi \varepsilon)$.

Namely, this matrix is assumed to be sufficiently close to the unit matrix $I_n$, in particular, its diagonal elements should be close to one. This is measured by the operator norm of $\text{Var}(\tilde{\varepsilon}) - I_n$ and by deviations of the individual variances $\mathbb{E}\tilde{\varepsilon}_i^2$ from one:

$$\delta_1 \overset{\text{def}}{=} \|\text{Var}(\tilde{\varepsilon}) - I_n\|_{\text{op}},$$

$$\delta_\varepsilon \overset{\text{def}}{=} \max_i |\mathbb{E}\tilde{\varepsilon}_i^2 - 1|.$$  

(3.6)

In particular, in the case of homogeneous errors $\Sigma = \sigma^2 I_n$ and the smoothing operator $\Pi$ as a $p$-dimensional projector, it holds

$$\text{Var}(\tilde{\varepsilon}) = (I_n - \Pi)^2 = I_n - \Pi \leq I_n,$$

$$\delta_1 = \|\text{Var}(\tilde{\varepsilon}) - I_n\|_{\text{op}} = \|\Pi\|_{\text{op}} = 1,$$

$$\delta_\varepsilon = \max_i |\mathbb{E}\tilde{\varepsilon}_i^2 - 1| = \max_i |\Pi_{ii}|.$$

One can check that $\Pi_{ii} \approx \sqrt{p/n}$ for typical smoothing operators like local average or kernel smoothing. Similar bounds with an additional constant can be established for general regular noise $\varepsilon$ and a general smoothing operator $\Pi$.

**Regularity of the smoothing operator $\Pi$** is required in Theorem 3.2. This condition will be expressed via the norm of the rows $T_i^\top$ of the matrix $\Upsilon \overset{\text{def}}{=} \Sigma^{-1/2} \Pi \Sigma^{1/2}$ fulfill

$$\|T_i^\top\| \leq \delta_\psi, \quad i = 1, \ldots, n.$$  

(3.7)

This condition is in fact very close to the design regularity condition (3.4). To see this, consider the case of a homogeneous noise with $\Sigma = \sigma^2 I_n$ and $\Pi = \psi^\top(\psi\psi^\top)^{-1}\psi$. Then $\Upsilon = \Pi$ and (3.4) implies

$$\|\Upsilon_i^\top\| = \|\psi^\top(\psi\psi^\top)^{-1}\psi_i\| = \|((\psi\psi^\top)^{-1/2}\psi_i\| \leq \delta_\psi.$$
In general one can expect that (3.7) is fulfilled with some other constant which however, is of the same magnitude as $\delta_\Psi$. For simplicity, we use the same symbol.

3.2 Bootstrap validation. Range of applicability

This section states the main results justifying the proposed bootstrap procedure. They claim that the joint distribution $Q^b$ of the bootstrap stochastic components $\xi_{m,m^\circ}^b$ for $m > m^\circ$ nicely reproduces the underlying distribution $Q$ of the $\xi_{m,m^\circ}$'s, and hence, all the probabilistic results obtained in Section 2 for known noise continue to apply after bootstrap parameter tuning. In the next result, we give a bound on the total variation distance $\|Q - Q^b\|_{TV}$ between $Q$ and $Q^b$.

**Theorem 3.1.** Let $Y = f^* + \varepsilon$ be a Gaussian vector in $\mathbb{R}^n$ with independent components, $Y \sim N(f^*, \Sigma)$ for $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_n^2)$. Let also $\Psi$ be a $p \times n$ feature matrix such that the $p \times p$-matrix $S = \Psi \Sigma \Psi^\top$ is non-degenerated. For a given presmoother operator $\Pi: \mathbb{R}^n \rightarrow \mathbb{R}^n$, assume that $\delta_1$ from (3.6) satisfies $\delta_1 \leq 1$. Let $Q = \mathcal{L}(\xi_{m,m^\circ}, m, m^\circ \in M)$ and let $Q^b$ be the joint conditional distribution of the bootstrap stochastic terms $\xi_{m,m^\circ}^b$ for $m, m^\circ \in M$ given the data $Y$. Then it holds on a random set $\Omega_2(x)$ with $\mathbb{P}(\Omega_2(x)) \geq 1 - 3e^{-x}$:

$$\|Q - Q^b\|_{TV} \leq \frac{1}{2} \Delta_2(x),$$

(3.8)

$$\Delta_2(x) \overset{\text{def}}{=} 2 \sqrt{\delta_\Psi^2 p x_n + \sqrt{\delta_\varepsilon^2 p} + \sqrt{\|B\|_4^4 p + 4 \delta_\Psi^2 \|B\|_p} (1 + \sqrt{x}).$$

where $x_n = x + \log(n)$, the bias $B$ is given by (3.5) and $\delta_1, \delta_\varepsilon$ by (3.6).

The result (3.8) gives us a way to control differences $Q(A) - Q^b(A)$ for fixed sets $A$. To justify the propagation property for the bootstrap-based set of critical values $z_{m,m^\circ}^b(x + q_{m^\circ})$, given according to (3.1), (3.2), and (3.3) with $\hat{Y} = Y - \Pi Y$, we also need to take into account the $Y$-dependence of $z_{m,m^\circ}^b(x + q_{m^\circ})$. This is done by the following theorem.

**Theorem 3.2.** Assume the conditions of Theorem 3.1, and let the rows $\gamma_i^\top$ of the matrix $Y \overset{\text{def}}{=} \Sigma^{-1/2} \Pi \Sigma^{1/2}$ satisfy (3.7). Then for each $m^\circ \in M$

$$\mathbb{P}\left(\max_{m > m^\circ} \left\{ \|\xi_{m,m^\circ} - z_{m,m^\circ}^b(x + q_{m^\circ})\| \geq 0 \right\} \right) \leq 6e^{-x} + \sqrt{p} \Delta_0(x),$$

(3.9)

where with $x_n = x + \log(n)$ and $x_p = x + \log(2p)$

$$\Delta_0(x) \overset{\text{def}}{=} \|B\|_\infty^2 + \delta_\Psi^2 \|B\|\sqrt{2x} + 2\delta_\varepsilon x_n + \delta_\Psi^2 x_n + 2\delta_\Psi \sqrt{x_p} + 2\delta_\varepsilon^2 x_p.$$
The SmA procedure also involves the values \( p_{m,m^o}, \) which are unknown and depend on the noise \( \varepsilon. \) The next result shows the bootstrap counterparts \( p_{m,m^o}^\flat \) can be well used in place of \( p_{m,m^o}. \)

**Theorem 3.3.** Assume the conditions of Theorem 3.1. Then it holds on a set \( \Omega_1(x) \) with \( P(\Omega_1(x)) \geq 1 - 3e^{-x} \) for all pairs \( m < m^o \in M \)

\[
\frac{p_{m,m^o}^{\flat}}{p_{m,m^o}} - 1 \leq \Delta_p,
\]

where \( p_{m,m^o}^{\flat} = E^\flat \| \xi_{m,m^o}^{\flat} \|^2, \) \( p_{m,m^o} = E\| \xi_{m,m^o} \|^2, \) and \( x_M = x + 2 \log(|M|). \)

The above results immediately imply all the oracle bounds for probabilistic loss of Section 2 with the obvious correction of the error terms.

Now we discuss the sense of the required conditions for bootstrap validity. Our results are only meaningful and the bootstrap approximation is accurate if the values \( \Delta_2(x) \) and \( \sqrt{p} \Delta_0(x) \) are small. One easily gets

\[
\Delta_2(x) \asymp \sqrt{p} \Delta_0(x) \leq C p^{1/2} (\| B \|^2_\infty + \delta_\psi^2 \| B \| + \delta_\psi + \delta_\varepsilon),
\]

where \( \delta \psi^2 \) is a generic notation for absolute constants and log-terms like \( x_n, x_p \) etc. So, keeping the errors of bootstrap approximation small requires that the values \( \delta_\psi^2 p, \delta_\varepsilon^2 p, \| B \|^4_\infty p, \) and \( \delta_\psi^2 \| B \| \) are sufficiently small. Now we spell this condition in the typical situation with \( \delta_\psi \asymp \sqrt{p/n} \) and \( \delta_\varepsilon \asymp \sqrt{p/n}. \) Then we need that \( p^2 \log(n)/n \) is small. Further, the bias component does not destroy the bootstrap validity result if the values \( \| B \|^4_\infty p \) and \( p n^{-1} \| B \| \leq p n^{-1/2} \| B \|_\infty \) are small. If \( f^* \) is Hölder-smooth with the parameter \( s: \)

\[
\| B \|_\infty \leq C p^{-s}
\]

then the bootstrap procedure is justified for \( s > 1/4 \) if \( p = p_n \to \infty \) but \( p_n^2/n \to 0 \) as \( n \to \infty. \) We state one asymptotic result of this sort.

**Corollary 3.4.** Assume the conditions of Theorem 3.2 and let \( p = p_n \) fulfill \( p_n^2 \log(n)/n \to 0 \) as \( n \to \infty, \) and (3.10) hold for \( s > 1/4. \) Then the results of Theorem 3.1 and 3.2 apply with a small value \( \Delta_n = (\sqrt{p_n} \Delta_0(x_n)) \vee \Delta_2(x_n) \to 0 \) as \( n \to 0. \)

### 4 Simulations

This section illustrates the performance of the proposed procedure by means of simulated examples. We consider a regression problem for an unknown univariate function on \([0,1]\)
We also check the sensitivity of the method to the choice of the presmoothing parameter \( m^\dagger \).

We use a uniform design on \([0, 1]\) and the Fourier basis \( \{ \psi_j(x) \}_{j=1}^\infty \) for approximation of the regression function \( f \) which is modelled in the form

\[ f(x) = c_1 \psi_1(x) + \ldots + c_p \psi_p(x), \]

where the \( (c_j)_{1 \leq j \leq p} \) are chosen randomly: with \( \gamma_j \) i.i.d. standard normal

\[ c_j = \begin{cases} 
\gamma_j, & 1 \leq j \leq 10, \\
\gamma_j/(j-10)^2, & 11 \leq j \leq 200. 
\end{cases} \]

The noise intensity grows from low to high as \( x \) increases to one. We use \( n_{\text{sim-bs}} = n_{\text{sim-theo}} = n_{\text{sim-calib}} = 1000 \) samples for computing the bootstrap marginal quantiles and the theoretical quantiles and for checking the calibration condition. The maximal model dimension is \( M = 37 \) and we also choose \( m^\dagger = 20 \). The calibration is run with \( x = 2 \) and \( \beta = 1 \).

We start by considering examples for \( W = \psi_{11}^\top \), i.e. the estimation of the whole function vector with prediction loss. One can see in Figure 4.1 three examples with different intensity of the noise term comparing the Bootstrap-method to the oracle estimator and
the known-variance SmA-Method. Figure 4.2 illustrates the dependence of the choice of
the estimated dimension on our calibration dimension \( m^\dagger \) and the sample size \( n \). We see
that in the specific example we are considering, the sensitivity of the chosen dimension
\( \hat{m} \) on \( m^\dagger \) decreases very fast. In the case \( n = 200 \), we have no variation in the choice
of \( \hat{m} \) with respect to \( m^\dagger \). The oracles are respectively \( m^* = 12 \) for \( n = 100, 200 \) and
\( m^* = 10 \) for \( n = 50 \). We also want to compare the true quantiles and their bootstrap

![Graphs](Image)

Figure 4.2: The first three plots show an exemplary function with \( n = 50, 100, 200 \)
observations. The right plot shows the \( \hat{m} \) chosen by the Bootstrap-SmA-Method as a
function of the calibration dimension \( m^\dagger \) and the number of observations.

substitute. Figure 4.3 plots the ratios of quantiles for all possible comparisons \((m_1, m_2)\)
for the same function as before. Here we see that there is, as one would expect, still sig-
nificant variation in the quantile ratios for small differences \(|m_1 - m_2|\). Nonetheless the
method works very well as seen in Fig. 4.2, but the variability in the ratios implies the
possibility to stabilize the procedure even more by introducing some smoothing scheme
for the quantiles.

Figure 4.4 again demonstrates the dependence of the ratios on \( m^\dagger \). It is remarkable
that the ratio is varying very slowly above \( m^* = 12 \). We also give the results on the
simulation of \( n_{\text{hist}} = 100 \) repeated applications of the method to the same true underlying
function observed with different realizations of the errors in Figure 4.5.

The case of the estimation of the first derivative is similar. Figure 4.6 shows the
numerical results for estimation of the derivative in the same model as above. One
can see that the bootstrap-version of the SmA-procedure is again competitive with the
procedure based on a known noise structure and the method does a good job of mimicking
the oracle.

One can conclude that the proposed procedure is really universal and demonstrates
a very good performance in various settings.
Figure 4.3: Ratio of quantiles $|\hat{s}_{m_1,m_2}^b/\hat{s}_{m_1,m_2}|^2$ for $m^\dagger = 20$ and $n = 200$ with the data and true function as in Fig. 4.2.

Figure 4.4: Maximal, minimal and mean ratio of the bootstrap and theoretical tail functions at $x = 2$, $|\hat{s}_{m_1,m_2}^b/\hat{s}_{m_1,m_2}|^2$ as a function of $m^\dagger$.

Figure 4.5: In the left plot, the true function and observed values are plotted for one realization together with the oracle estimator, the known-variance SmA-Estimator (SmA-Est.) and the Bootstrap-SmA-Estimator (SmA-BS-Est.). The numbers in parentheses indicate the chosen model dimension. In the right plot, histograms for the selected model are given for the bootstrap (BS) and the known-variance method (MC) for repeated observations of the same underlying function with a simulation size $n_{\text{hist}} = 100$. 
Figure 4.6: The upper left plot shows the true derivative, the oracle estimator, the known-variance SmA-Estimator (SmA-Est.) and the Bootstrap-SmA-Estimator (SmA-BS-Est.). The upper right plot shows the true function and the observations and in the lower plot one can find the standard deviation of the errors.

A Proofs

The appendix collects the proofs of announced results.

A.1 Proof of Theorem 2.1

The propagation property (2.13) claims that the oracle model $m^*$ will be accepted with high probability. This yields that the selected model is not larger than $m^*$, that is, $\hat{m} \leq m^*$ with a probability at least $1 - e^{-x}$. Below we consider only this event. Let $m \in M^{-}(m^*)$. Acceptance of $m$ requires in particular that $\mathbb{T}_{m^*, m} \leq \bar{z}_{m^*, m}$. The representation $\mathbb{T}_{m^*, m} = \|b_{m^*, m} + \xi_{m^*, m}\|$ implies

$$\mathbb{P}(\mathbb{T}_{m^*, m} < \bar{z}_{m^*, m}) \leq \mathbb{P}(\|\xi_{m^*, m}\| > \|b_{m^*, m}\| - \bar{z}_{m^*, m}).$$

Under (2.14) this yields

$$\mathbb{P}(m \text{ is accepted}) \leq \mathbb{P}(\|b_{m^*, m} + \xi_{m^*, m}\| \leq \bar{z}_{m^*, m}) \leq \mathbb{P}(\|\xi_{m^*, m}\| \geq z_{m^*, m}(x)) \leq e^{-x}. \quad (A.1)$$

If the lower bound on the bias is fulfilled for all $m \in M^c$, then (A.1) helps to bound the probability of the event $\{\hat{m} \in M^c\}$:

$$\mathbb{P}(\hat{m} \in M^c) \leq \sum_{m \in M^c} \mathbb{P}(\|b_{m^*, m} + \xi_{m^*, m}\| < \bar{z}_{m^*, m}) \leq \sum_{m \in M^c} e^{-x} \leq e^{-x}.$$
Therefore, the probability that the SmA-selector picks up a value $m > m^*$ or $m \in M^c$ is very small:

$$P(\hat{m} \in M^+(m^*) \cup M^c) \leq 2e^{-x}.$$ 

It remains to study the case when $\hat{m} = m \in M^o = M^-(m^*) \setminus M^c$. We can use that $\hat{m}$ is accepted, which implies by definition

$$T_{m^*,m} = \|\tilde{\phi}_m - \tilde{\phi}_{m^*}\| \leq \delta_{m^*,m}.$$ 

This yields (2.15). The bound (2.17) now follows by the triangle inequality.

### A.2 Proof of Proposition 2.2

Below we use the deviation bound (D.2) for a Gaussian quadratic form from Theorem D.1. Note that similar results are available for non-Gaussian quadratic forms under exponential moment conditions; see e.g. Spokoiny (2012). The result (D.2) combined with the Bonferroni correction $q_m = \log(|M^+(m^*)|) \leq \log(|M|)$ yields the following upper bound for the critical values $\delta_{m,m^o}$:

$$\delta_{m,m^o} \leq z_{m,m^o}(x + q_m) + \beta \sqrt{p_{m,m^o}} \{x + \log(|M^+(m^*)|)\}$$

For the payment for adaptation $\delta_{m^*,m}$, the result (A.2) and the monotonicity condition $p_{m^*,m} \leq p_{m^*,m_0} \leq p_{m^*}$ and $\lambda_{m^*,m} \leq \lambda_{m^*,m_0} \leq \lambda_{m^*}$ imply the following upper bound:

$$\delta_{m^*,m} \leq (1 + \beta)\sqrt{p_{m^*,m_0}} + \sqrt{2\lambda_{m^*,m_0}} \{x + \log(|M^-(m^*)|)\}$$

which yields the claim.

### A.3 Proof of Theorem 2.3

The result will be proved in two steps. First we bound the risk on the set $\hat{m} > m^*$:

$$IE\{\|\hat{\phi} - \phi^*\|^2 \mathbb{I}(\hat{m} > m^*)\} \leq 2\pi_m, R_{m^*}.$$ (A.3)

Then we consider the region $\hat{m} < m^*$ and prove an oracle inequality

$$\|\hat{\phi} - \tilde{\phi}_m\| \mathbb{I}(\hat{m} < m^*) \leq \delta_{m^*}.$$ (A.4)
and the oracle bound (2.25). We start by proving (A.3). Let us fix \( m \in \mathcal{M}^+(m^*) \) and \( m' \geq m \). The definition (2.18) of the oracle \( m^* \) and the formula (2.22) for the critical value \( \delta_{m',m(-1)} \) implies for the test statistic \( T_{m',m(-1)} = \|\xi_{m',m(-1)} + b_{m',m(-1)}\| \)

\[
\{ T_{m',m(-1)} > \delta_{m',m(-1)} \} \subseteq \{ \|\xi_{m',m(-1)}\| > z_{m',m(-1)}(z_{m(-1)}) \}.
\]

Now we can bound the risk of \( \hat{\phi} \) on the set \( \hat{m} > m^* \). We use that for \( \hat{m} = m > m^* \) in view of (2.19)

\[
\|\hat{\phi} - \phi^*\|^2 = \|\hat{\phi}_m - \phi^*\|^2 = \|\xi_m + b_m\|^2 \\
\leq 2\|\xi_m\|^2 + 2\|b_m\|^2 \leq 2\|\xi_m\|^2 + 2\|b_{m^*}\|^2
\]

and it holds by (2.21) and monotonicity \( p_m > p_{m^*} \)

\[
\mathbb{E}\{\|\hat{\phi} - \phi^*\|^2 \mathbb{I}(\hat{m} > m^*)\} \\
\leq 2 \sum_{m \in \mathcal{M}^+(m^*)} \mathbb{E}\{\|\xi_m\|^2 + \|b_{m^*}\|^2 \mathbb{I}(m = \hat{m})\} \\
\leq 2 \sum_{m \in \mathcal{M}^+(m^*)} \mathbb{E}\{\|\xi_m\|^2 + \|b_{m^*}\|^2 \mathbb{I}(m(-1) \text{ is rejected})\} \\
= 2 \sum_{m \in \mathcal{M}^+(m^*)} \mathbb{E}\left[\left(\|\xi_m\|^2 + \|b_{m^*}\|^2\right) \mathbb{I}\left(\max_{m' \in \mathcal{M}^+(m)} \left\{\|\xi_{m',m(-1)}\| - z_{m',m(-1)}(z_{m})\right\} > 0\right)\right] \\
\leq 2 \sum_{m \in \mathcal{M}^+(m^*)} \alpha_m (p_m + \|b_{m^*}\|^2) \leq 2\overline{\alpha}_{m^*}(p_{m^*} + \|b_{m^*}\|^2) = 2\overline{\alpha}_{m^*}\mathcal{R}_{m^*}.
\]

Here we have used that (2.24) and \( p_m \geq p_{m^*} \) imply \( \sum_{m \in \mathcal{M}^+(m^*)} \alpha_m \leq \overline{\alpha}_{m^*} \). This completes the proof of (A.3).

In the situation when \( \hat{m} = m < m^* \), we can use the stability property: as \( m \) is accepted, it holds

\[
\|\hat{\phi}_m - \hat{\phi}_{m^*}\| \mathbb{I}(\hat{m} = m) \leq \delta_{m^*,m},
\]

which implies (A.4) by definition of \( \delta_{m^*,m} \). This yields

\[
\mathbb{E}\|\hat{\phi} - \phi^*\|^2 \leq 2\overline{\alpha}_{m^*}\mathcal{R}_{m^*} + \mathbb{E}\{\|\hat{\phi} - \phi^*\|^2 \mathbb{I}(\hat{m} < m^*)\} \\
\leq 2\overline{\alpha}_{m^*}\mathcal{R}_{m^*} + \mathbb{E}(\|\hat{\phi}_{m^*} - \phi^*\| + \delta_{m^*,m})^2 \\
\leq 2\overline{\alpha}_{m^*}\mathcal{R}_{m^*} + (\mathcal{R}_{m^*}^{1/2} + \delta_{m^*,m})^2
\]

as required.
A.4 Proof of Proposition 2.4

Observe first that the choice $\alpha_m = (p_m/p_{m0})^{-1-a}$ yields

$$\sum_{m \in M^+ (m^*)} \alpha_m p_m \leq p_{m0}^{1+a} \sum_{m \in M^+ (m^*)} p_m^{-a} \leq C p_{m0}^{-a} p_{m0}^{1+a} = C \overline{\alpha}_{m^*} p_{m^*},$$

with $\overline{\alpha}_{m^*} = C (p_{m0}/p_{m^*})^{1+a}$.

For any random vector $\xi$ with $\text{Var}(\xi) = B$ and $p = \text{tr}(B)$ and any random event $A$, it holds

$$\mathbb{E} \left[ p^{-1} \| \xi \|^2 | A \right] \leq \left\{ 1 + p^{-2} \text{Var}(\| \xi \|^2) \right\}^{1/2} p^{1/2} |A|.$$  \hspace{1cm} (A.5)

Indeed, the Cauchy-Schwartz inequality implies

$$\mathbb{E} \left\{ p^{-1} \| \xi \|^2 | A \right\} \leq \mathbb{E}^{1/2} \{ p^{-1} \| \xi \|^2 \} |A| = \left\{ 1 + p^{-2} \text{Var}(\| \xi \|^2) \right\}^{1/2} p^{1/2} |A|.$$  

Moreover, in the Gaussian case $\xi \sim N(0, B)$ with $\|B\|_{op} \leq 1$, it holds $\text{Var}(\| \xi \|^2) \leq 2p$. If $p$ is large then $\text{Var}(\| \xi \|^2)/p^2$ is small. In general $\text{Var}(\| \xi \|^2)/p^2 \leq 2$.

Result (A.5) and the choice $\alpha_m = \sqrt{3} p_m^{-1-a}$ allow to specify an upper bound on $x_m$. Namely, the choice $x_m = C \log(p_m)$ ensures the propagation condition (2.20). To see this, fix $m$ and $m' \geq m$. Let

$$A'_m(x) \overset{\text{def}}{=} \mathbb{I} \left( \max_{m'' \in M^+(m)} \{ \| \xi_{m'',m} \| - \sqrt{p_{m'',m}} - \sqrt{2 \lambda_{m'',m}} \{ x + \log(|M|) \} > 0 \} \right).$$

The arguments after Lemma D.1 with $x_{m(-1)} = 2(1 + a) \log(p_m)$ and (A.5) imply

$$\mathbb{E} \left[ p_m^{-1} \| \xi_m \|^2 | A'_m(x_{m(-1)}) \right] \leq \sqrt{3} e^{-(1+a) \log(p_m)} = \sqrt{3} p_m^{1-a}$$

and by (2.22)

$$z_{m,m^*} \leq \sqrt{p_{m,m^*}} + \sqrt{2 \lambda_{m,m^*}} \{ (1 + a) \log(p_{m^*+1}) + \log(|M|) \}.$$  

This implies the upper bound (2.28) on the payment for adaptation $\overline{z}_{m^*}$.

A.5 Proof of Theorem 3.1

Any statement on the use of bootstrap-tuned parameters faces the same fundamental problem: the bootstrap distribution is random and depends on the underlying sample. When we use such values for the original procedure, we have to account for this dependence. The statement of Theorem 3.1 is even more involved due to the presmoothing
step and multiplicity correction (3.3). The proof will be split into a couple of steps. First we evaluate the effect of the presmoothing bias and variance and reduce the study to an artificial situation where one uses the errors \( \epsilon_i \) for resampling in place of the residuals \( \tilde{Y}_i \). Then we compare \( Q \) and \( Q^b \) using the Pinsker inequality.

Below we write \( \Psi \) in place of \( \Psi_M \), where \( M \) is the largest model in the collection. This does not conflict with our general setup, it is implicitly assumed that the largest model coincides with the original one. By \( p \) we denote the corresponding parameter dimension, that is, \( \Psi \) is a \( p \times n \) matrix. Further, the feature matrix \( \Psi_m \) can be written as the product \( \Psi_m = \Pi_m \Psi \), where \( \Pi_m \) is the projector on the subspace of the feature space spanned by the features from the model \( m \): \( \Pi_m = (\Psi_m \Psi_m^\top)^{-1} \Psi_m \). This allows to represent each estimator \( \tilde{\phi}_m \) in the form

\[
\tilde{\phi}_m = W \tilde{\theta}_m = W S_m Y = W (\Psi_m \Psi_m^\top)^{-1} \Psi_m Y = T_m \Psi Y
\]

This implies the following representation of the stochastic components \( \xi_{m,m^o} \):

\[
\xi_{m,m^o} = T_m \Psi \epsilon = T_m \Psi \nabla, \quad T_m \Psi = T_m - T_{m^o},
\]

where \( \nabla = \Psi \epsilon \). One can say that each stochastic vector \( \xi_{m,m^o} \) is a linear function of the vector \( \nabla \). A similar representation holds true in the bootstrap world:

\[
\xi_{m,m^o}^b = T_m \Psi \text{diag}(\tilde{Y}) w^b = T_m \Psi \nabla^b, \quad \nabla^b = \Psi \text{diag}(\tilde{Y}) w^b.
\]

Here the original errors \( \epsilon \) are replaced by their bootstrap surrogates \( \epsilon^b = \text{diag}(\tilde{Y}) w^b \). Therefore, it suffices to compare the distribution of \( \nabla = \Psi \epsilon \) with the conditional distribution of \( \nabla^b = \Psi \text{diag}(\tilde{Y}) w^b \) given \( Y \). Then the results will be automatically extended to any deterministic mapping of these two vectors.

Normality of the errors \( \epsilon_i \sim \mathcal{N}(0,\sigma^2_i) \) implies that \( \nabla = \Psi \epsilon \) is also normal zero mean:

\[
\nabla \sim \mathcal{N}(0,S), \quad S \overset{\text{def}}{=} \Psi \Sigma \Psi^\top, \quad \Sigma = \text{Var}(\epsilon) = \text{diag}(\sigma^2_1,\ldots,\sigma^2_n).
\]

Similarly we can use standard normality of the bootstrap weights \( w^b_i \). Given the data \( Y \), the vector \( \nabla^b \) is conditionally normal zero mean with the conditional variance

\[
S^b \overset{\text{def}}{=} \text{Var}^b(\nabla^b) = \Psi \text{diag}(\tilde{Y}_1^2,\ldots,\tilde{Y}_n^2) \Psi^\top = \Psi \text{diag}(\tilde{Y} \cdot \tilde{Y}) \Psi^\top.
\]

Therefore, the problem is reduced to comparing two \( p \)-dimensional Gaussian distributions with different covariance matrices. Equivalently, we have to bound the value \( \Delta = \sqrt{\text{tr}(B^2)} \) for a random \( p \times p \) matrix \( B \) given by

\[
B \overset{\text{def}}{=} S^{-1/2} (S^b - S) S^{-1/2}.
\]
Define a $p \times n$ matrix $\mathbf{U} = S^{-1/2} \Psi \Sigma^{1/2}$ so that $\mathbf{U} \mathbf{U}^\top = \mathbf{I}_p$. We will use the decomposition

$$
\Sigma^{-1/2} \mathbf{Y} = \Sigma^{-1/2} (\mathbf{Y} - \Pi \mathbf{Y}) + \Sigma^{-1/2} (\mathbf{f}^* - \Pi \mathbf{f}^*) = \eta + \mathbf{B}
$$

with

$$
\eta \overset{\text{def}}{=} \Sigma^{-1/2} (\varepsilon - \Pi \varepsilon), \quad \mathbf{B} \overset{\text{def}}{=} \Sigma^{-1/2} (\mathbf{f}^* - \Pi \mathbf{f}^*).
$$

(A.6)

With the matrix $\mathbf{B}$ can now be represented as

$$
\mathbf{B} = \mathbf{U} \text{diag} \left\{ (\eta + \mathbf{B}) \cdot (\eta + \mathbf{B}) - I_n \right\} \mathbf{U}^\top = \mathbf{U} \text{diag} \left\{ (\eta + \mathbf{B}) \cdot (\eta + \mathbf{B}) - \eta \cdot \eta \right\} \mathbf{U}^\top \overset{\text{def}}{=} \mathbf{B}_1
$$

$$
+ \mathbf{U} \text{diag} \left\{ \eta \cdot \eta - \mathbb{E}(\eta \cdot \eta) \right\} \mathbf{U}^\top \overset{\text{def}}{=} \mathbf{B}_2
$$

$$
+ \mathbf{U} \text{diag} \left\{ \mathbb{E}(\eta \cdot \eta) - I_n \right\} \mathbf{U}^\top \overset{\text{def}}{=} \mathbf{B}_3.
$$

(A.7)

The first term $\mathbf{B}_1$ in this decomposition expresses the impact of the bias $\mathbf{B}$ remaining after presmoothing, the last two terms $\mathbf{B}_2$ and $\mathbf{B}_3$ measure the change of the noise covariance due to presmoothing. The triangle inequality in the Frobenius norm $\|\mathbf{B}\|_\text{Fr} \overset{\text{def}}{=} \sqrt{\text{tr}(\mathbf{B}^2)}$ and bounds from Propositions E.6, E.7, and E.8 with $\mathbf{U} \mathbf{U}^\top = \mathbf{I}_p$ and $q = q_2 = \text{tr}(\mathbf{U} \mathbf{U}^\top) = p$ imply on a random set $\Omega_2(x) = \Omega_{12}(x) \cup \Omega_{22}(x)$ with $\mathbb{P}(\Omega_2(x)) \geq 1 - 2e^{-x}$

$$
\|\mathbf{B}\|_\text{Fr} \leq \|\mathbf{B}_1\|_\text{Fr} + \|\mathbf{B}_2\|_\text{Fr} + \|\mathbf{B}_3\|_\text{Fr}
$$

$$
\leq \Delta_1(x) + \Delta_2(x) + \Delta_3(x)
$$

$$
= 2 \sqrt{\delta_2^2 p (x + \log(n))} + \sqrt{\delta_2^2 p} + \sqrt{\|\mathbf{B}\|_\infty^4 p} + 4 \delta_2^2 \|\mathbf{B}\| (1 + \sqrt{x}).
$$

This proves (3.8) in view of Pinsker’s Lemma F.1 with $b = b^b = 0$.

### A.6 Proof of Theorem 3.2

The result of Theorem 3.1 justifies the bootstrap-phenomenon, namely it explains why the known bootstrap distribution can be used as a proxy for the unknown error distribution. However, it cannot be applied directly to (3.9) because the quantities $z_{\mathbf{m},\mathbf{m}^c}(x)$ and $\tilde{d}_{\mathbf{m}^c}$ are random and depend on the original data. This especially concerns the multiplicity correction $q_{\mathbf{m}^c}$ which is based on the joint distribution of the vectors $\xi_{\mathbf{m},\mathbf{m}^c}$ from (3.1) and is defined in (3.3). The latter distribution is a random measure in the bootstrap world which is normal conditioned on the original sample. To cope with the problem of this cross-dependence, we apply the statement of Theorem B.1 in the Appendix. The underlying idea is to use geometric arguments to sandwich the random probability in (3.3) in two deterministic probabilities. Then the error of bootstrap approximation can
again be bounded by using the Pinsker inequality. The statement of Theorem 3.2 can be derived from Theorem B.1 if an operator norm bound \( \|B\|_{op} \) is available. Note that Theorem 3.1 only requires a bound for the Frobenius norm. By Proposition E.9, it holds with \( \delta_n = \delta_\psi \), \( x_n = x + \log(n) \), and \( x_p = x + 2 \log(p) \):

\[
\|B\|_{op} \leq \Delta_{op}(x),
\]

\[
\Delta_{op}(x) \overset{\text{def}}{=} \|B\|_\infty + \delta^2 \|B\| \sqrt{2x} + 2 \delta_\psi x_p^{1/2} + 2 \delta_\psi x_p + 2 \delta_\psi x_n + \delta^2 x_n.
\]

The result of the theorem follows now by Theorem B.1.

### A.7 Proof of Theorem 3.3

For a fixed pair \( m > m^0 \) from \( \mathcal{M} \), consider \( p^{\flat}_{m,m^0} = \mathbb{E} \|\xi_{m,m^0}\|^2 \) and \( p_{m,m^0} = \mathbb{E} \|\xi_{m,m^0}\|^2 \). As \( \text{diag}(\bar{Y}) \) and \( \Sigma \) are diagonal matrices, the definitions (3.1) and (A.6) imply

\[
\xi_{m,m^0} = \mathbb{K}_{m,m^0} \text{ diag}(\bar{Y}) w^{\flat} = \mathbb{K}_{m,m^0} \Sigma^{1/2} \Sigma^{-1/2} \text{ diag}(\bar{Y}) w^{\flat}
\]

\[
= \mathbb{U}_{m,m^0} \text{ diag}(\eta + B) w^{\flat},
\]

where \( \mathbb{U}_{m,m^0} \overset{\text{def}}{=} \mathbb{K}_{m,m^0} \Sigma^{1/2} \). It holds for \( p^{\flat}_{m,m^0} \)

\[
p^{\flat}_{m,m^0} = \mathbb{E} \|\xi_{m,m^0}\|^2 = \text{tr} \left( \mathbb{U}_{m,m^0} \text{ diag} \{ (\eta + B) \cdot (\eta + B) \} \mathbb{U}_{m,m^0}^T \right)
\]

while \( \xi_{m,m^0} = \mathbb{K}_{m,m^0} \Sigma^{1/2} \Sigma^{-1/2} \varepsilon \) and

\[
p_{m,m^0} = \mathbb{E} \|\xi_{m,m^0}\|^2 = \text{tr} \left( \mathbb{U}_{m,m^0} \mathbb{U}_{m,m^0}^T \right).
\]

As we are interested in the ratio \( p^{\flat}_{m,m^0} / p_{m,m^0} \), one can assume without loss of generality that \( \|\mathbb{U}_{m,m^0} \mathbb{U}_{m,m^0}^T\|_{op} = 1 \) and \( p_{m,m^0} \geq 1 \). Now we again apply the decomposition (A.7). The bounds (E.14) of Proposition E.6, (E.17) of Proposition E.7, and (E.19) of Proposition E.8 imply on a set \( \Omega_{m,m^0}(x) \) with \( P(\Omega_{m,m^0}(x)) \geq 1 - 3e^{-x} \)

\[
\left| \frac{p^{\flat}_{m,m^0}}{p_{m,m^0}} - 1 \right| \leq \|B\|_\infty + 4x^{1/2} \delta^2 \|B\| + 4x^{1/2} \delta_n + 4x \delta^2 + \delta_n + \delta_\varepsilon.
\]

The choice of \( x = x_M = x + 2 \log(|\mathcal{M}|) \) ensures a uniform bound for all pairs \( m > m^0 \) from \( \mathcal{M} \).

### B Random multiplicity correction

Suppose that \( V^{\flat} \) is a random positive symmetric \( p \times p \) matrix close to a deterministic matrix \( V \). Below we use the operator norm for quantifying the difference between \( V \)
and $V^b$: namely let with probability one
\[ \|V^{-1/2} V^b V^{-1/2} - I_p\|_{op} \leq \Delta_0. \] (B.1)

In what follows, $P = N(0, V)$ is the normal measure on $\mathbb{R}^p$ with mean zero and covariance $V$. Similarly $P^b$ is a random measure on $\mathbb{R}^p$ which is conditionally on $V^b$ normal with $P^b = N(0, V^b)$. Suppose that for each $m$ from a given set $M$ a linear mapping $T_m: \mathbb{R}^p \to \mathbb{R}^{p_m}$ is fixed. Given $x$, define for each $m \in M$ the corresponding tail function $z_m(x)$ by
\[ P\{u: \|T_m u\| \geq z_m(x)\} = e^{-x}. \] (B.2)

Also define a set $A(x)$ as
\[ A(x) \overset{\text{def}}{=} \left\{ u: \bigcap_{m \in M} \{\|T_m u\| \leq z_m(x)\} \right\}. \]

Similarly define $z_m^b(x)$ by (B.2) with $P^b$ in place of $P$, $m \in M$, and $A^b(x)$. Note that all these objects are random because $P^b$ is random. Finally, let $x^b_\alpha$ be the random quantity providing
\[ P^b(A^b(x^b_\alpha)) = 1 - \alpha. \] (B.3)

Below we try to address the question whether this random multiplicity correction based on (B.3) does a good job under $P$. This question leads to analysis of value $P(A^b(x^b_\alpha))$: the goal is in evaluating the difference
\[ P(A^b(x^b_\alpha)) - (1 - \alpha). \]

The analysis is non-trivial because $A^b(x)$ and $x^b_\alpha$ are random.

**Theorem B.1.** Let a random matrix $V^b$ satisfy (B.1) for a deterministic matrix $V$ and $\Delta_0 < 1/2$. Then it holds
\[ |P(A^b(x^b_\alpha)) - 1 + \alpha| \leq \sqrt{p} \Delta_0. \] (B.4)

**Proof.** The key property of $P^b = N(0, V^b)$ is that the random matrix $V^b$ concentrates around some deterministic matrix. Below we use this property in the bracketing form:
\[ V^- \leq V^b \leq V^+ \]

with
\[ V^- \overset{\text{def}}{=} (1 - \Delta_0)V, \quad V^+ \overset{\text{def}}{=} (1 + \Delta_0)V, \quad V^+ - V^- = 2\Delta_0 V. \] (B.5)
In other words, the random matrix $V^\flat$ can be sandwiched in two deterministic matrices $V^-$ and $V^+$. For the proof of (B.4) we use the following well known property of the Gaussian distribution.

**Lemma B.2.** Let $\mathcal{P}_1 \sim N(0, V_1)$ and $\mathcal{P}_2 \sim N(0, V_2)$ with $V_1 \leq V_2$. Then for any centrally symmetric star-shaped set $A$, it holds

$$\mathcal{P}_1(A) \geq \mathcal{P}_2(A).$$

**Proof.** The statement is trivial in the univariate case, the general case is obtained by integration over $A$ in polar coordinates. \hfill \square

Introduce two Gaussian measures $\mathcal{P}^- = N(0, V^-)$ and $\mathcal{P}^+ = N(0, V^+)$; see (B.5). Let $z_m^-(x)$ and $z_m^+(x)$ be the corresponding tail functions, and $A^-(x)$ and $A^+(x)$ - the corresponding sets. The identities (B.5) yield for each $x$ the relation

$$\mathcal{P}^+(A^+(x)) = \mathcal{P}^-(A^-(x)). \tag{B.6}$$

Lemma B.2 implies by (B.5) for any $x$

$$\mathcal{P}^+(A(x)) \leq \mathcal{P}^b(A(x)) \leq \mathcal{P}^-(A(x)). \tag{B.7}$$

The key step of the proof is given by the next lemma where we sandwich the random set $A^b(x^b)$ in two specially constructed deterministic sets.

**Lemma B.3.** Define the deterministic values $x^-_\alpha$ and $x^+_\alpha$ by the equations

$$\mathcal{P}^+(A^-(x^+_\alpha)) = 1 - \alpha,$$

$$\mathcal{P}^-(A^+(x^-_\alpha)) = 1 - \alpha. \tag{B.8}$$

Then

$$x^-_\alpha \leq x^b_\alpha \leq x^+_\alpha,$$

$$A^-(x^-_\alpha) \subseteq A^b(x^-_\alpha) \subseteq A^+(x^+_\alpha). \tag{B.9}$$

**Proof.** By Lemma B.2 the following inequalities and inclusions hold true for any $x$:

$$z_m^-(x) \leq z_m^b(x) \leq z_m^+(x),$$

$$A^-(x) \subseteq A^b(x) \subseteq A^+(x). \tag{B.10}$$

Now by definition (B.8) in view of (B.7) and (B.10)

$$\mathcal{P}^b(A^b(x^+_\alpha)) \geq \mathcal{P}^+(A^b(x^+_\alpha)) \geq \mathcal{P}^-(A^-(x^+_\alpha)) = 1 - \alpha,$$

$$\mathcal{P}^b(A^b(x^-_\alpha)) \leq \mathcal{P}^-(A^b(x^-_\alpha)) \leq \mathcal{P}^+(A^+(x^-_\alpha)) = 1 - \alpha.$$
This yields by monotonicity of $\mathbb{P}^b(A^b(x))$ in $x$ that $x^b_\alpha$ from (B.3) belongs to the interval $[x^-_\alpha, x^+_\alpha]$ and

$$
A^-(x^-_\alpha) \subseteq A^b(x^-_\alpha) \subseteq A^b(x^+_\alpha) \subseteq A^+(x^+_\alpha).
$$

This implies the result.

Now we are prepared to finalize the proof. The relations (B.9) and (B.6) imply

$$
\mathbb{P}^+(A^b(x^b_\alpha)) \leq \mathbb{P}^+(A^+((x^b_\alpha)) = \mathbb{P}^-(A^-((x^b_\alpha))).
$$

Furthermore, it holds by Pinsker’ inequality Corollary F.2 in view of (B.1) and (B.8)

$$
\mathbb{P}^-(A^-((x^+_\alpha))) \leq \mathbb{P}^+(A^-((x^+_\alpha))) + \sqrt{p} \Delta_0 \leq 1 - \alpha + \sqrt{p} \Delta_0.
$$

Similarly

$$
\mathbb{P}^-(A^b(x^-_\alpha)) \geq \mathbb{P}^-(A^b(x^b_\alpha)) = \mathbb{P}^+(A^b(x^-_\alpha))
$$

$$
\geq \mathbb{P}^+(A^b(x^-_\alpha)) - \sqrt{p} \Delta_0 = 1 - \alpha - \sqrt{p} \Delta_0.
$$

This implies (B.4) for the measure $\mathbb{P}$.

\[ \square \]

### C Deviation bounds for Gaussian law

This section collects some simple but useful facts about the properties of the multivariate standard normal distribution. Many similar results can be found in the literature, we present the proofs to keep the presentation self-contained. Everywhere in this section $\gamma$ means a standard normal vector in $\mathbb{R}^p$.

**Lemma C.1.** Let $\mu \in (0, 1)$. Then for any vector $\lambda \in \mathbb{R}^p$ with $\|\lambda\|^2 \leq p$ and any $r > 0$

$$
\log \mathbb{E}\{\exp(\lambda^\top \gamma) \mathbb{I}(\|\gamma\| > r)\} \leq -\frac{1-\mu}{2}r^2 + \frac{1}{2\mu}\|\lambda\|^2 + \frac{p}{2} \log(\mu^{-1}). \quad (C.1)
$$

Moreover, if $r^2 \geq 6p + 4\mu$, then

$$
\mathbb{E}\{\exp(\lambda^\top \gamma) \mathbb{I}(\|\gamma\| \leq r)\} \geq e^{\|\lambda\|^2/2(1 - e^{-x})}. \quad (C.2)
$$

**Proof.** We use that for $\mu < 1$

$$
\mathbb{E}\{\exp(\lambda^\top \gamma) \mathbb{I}(\|\gamma\| > r)\} \leq e^{-(1-\mu)r^2/2} \mathbb{E}\exp\{\lambda^\top \gamma + (1 - \mu)\|\gamma\|^2/2\}.
$$
It holds
\[ IE \exp\{\lambda^\top \gamma + (1 - \mu)\|\gamma\|^2/2\} = (2\pi)^{-p/2} \int \exp\{\lambda^\top \gamma - \mu\|\gamma\|^2/2\} d\gamma \]
\[ = \mu^{-p/2} \exp(\mu^{-1}\|\lambda\|^2/2) \]
and (C.1) follows.

Now we apply this result with \( \mu = 1/2 \). In view of \( IE \exp(\lambda^\top \gamma) = e^{\|\lambda\|^2/2} \), \( r^2 \geq 6p + 4x \), and \( 2 + \log(2) < 3 \), it follows for \( \|\lambda\|^2 \leq p \)
\[ e^{-\|\lambda\|^2/2} IE\{\exp(\lambda^\top \gamma) \mathbb{1}(\|\gamma\| \leq r)\} \geq 1 - \exp(-r^2/4 + p + (p/2) \log(2)) \geq 1 - \exp(-x) \]
which implies (C.2).

\section*{D Deviation bounds for Gaussian quadratic forms}

This section collects some deviation bounds for Gaussian quadratic forms. The next result explains the concentration effect of \( \gamma^\top B \gamma \) for a standard Gaussian vector \( \gamma \) and a symmetric matrix \( B \). We use a version from Laurent and Massart (2000).

\begin{result}
Let \( \gamma \) be a standard normal Gaussian vector and \( B \) be symmetric positive. Then with \( p = \text{tr}(B) \), \( v^2 = \text{tr}(B^2) \), and \( \lambda = \|B\|_{\text{op}} \), it holds for each \( x \geq 0 \)
\[ IP(\gamma^\top B \gamma > p + 2vx^{1/2} + 2\lambda x) \leq e^{-x}. \] (D.1)
\end{result}
This implies for any positive $B$

$$\mathbb{P}(\|B^{1/2}\gamma\| > p^{1/2} + (2\lambda x)^{1/2}) \leq e^{-x}. \quad (D.2)$$

Also

$$\mathbb{P}(\gamma^\top B\gamma < p - 2vx^{1/2}) \leq e^{-x}. \quad (D.3)$$

If $B$ is symmetric but non necessarily positive then

$$\mathbb{P}(\|\gamma^\top B\gamma - p\| > 2vx^{1/2} + 2\lambda x) \leq 2e^{-x}.$$

**Proof.** Normalisation by $\lambda$ reduces the statement to the case with $\lambda = 1$. Further, the standard rotating arguments allow to reduce the Gaussian quadratic form $\|\gamma\|^2$ to the chi-squared form:

$$\gamma^\top B\gamma = \sum_{j=1}^{p} \lambda_j \nu_j^2$$

with independent standard normal r.v.’s $\nu_j$. Here $\lambda_j \in [0,1]$ are eigenvalues of $B$, and $p = \lambda_1 + \ldots + \lambda_p$, $v^2 = \lambda_1^2 + \ldots + \lambda_p^2$. One can easily compute the exponential moment of $(\gamma^\top B\gamma - p)/2$: for each positive $\mu < 1$

$$\log \mathbb{E} \exp\{\mu(\gamma^\top B\gamma - p)/2\} = \frac{1}{2} \sum_{j=1}^{p} \{-\mu \lambda_j - \log(1 - \mu \lambda_j)\}. \quad (D.4)$$

**Lemma D.2.** Let $\mu \lambda_j < 1$ and $\lambda_j \leq 1$. Then

$$\frac{1}{2} \sum_{j=1}^{p} \{-\mu \lambda_j - \log(1 - \mu \lambda_j)\} \leq \frac{\mu^2 v^2}{4(1 - \mu)}.$$

**Proof.** In view of $\mu \lambda_j < 1$, it holds for every $j$

$$-\mu \lambda_j - \log(1 - \mu \lambda_j) = \sum_{k=2}^{\infty} \frac{(\mu \lambda_j)^k}{k} \leq \frac{(\mu \lambda_j)^2}{2} \sum_{k=0}^{\infty} (\mu \lambda_j)^k \leq \frac{(\mu \lambda_j)^2}{2(1 - \mu)} \leq \frac{(\mu \lambda_j)^2}{2(1 - \mu)}, \quad (D.5)$$

and thus

$$\frac{1}{2} \sum_{j=1}^{p} \{-\mu \lambda_j - \log(1 - \mu \lambda_j)\} \leq \sum_{j=1}^{p} \frac{(\mu \lambda_j)^2}{4(1 - \mu)} \leq \frac{\mu^2 v^2}{4(1 - \mu)}.$$
The next technical lemma is helpful.

**Lemma D.3.** For each $v > 0$ and $x > 0$, it holds

$$
\inf_{\mu > 0} \left\{ -\mu (vx^{1/2} + x) + \frac{\mu^2 v^2}{4(1 - \mu)} \right\} \leq -x.
$$

**Proof.** Let pick up

$$
\mu = 1 - \frac{1}{2x^{1/2}/v + 1} = \frac{x^{1/2}}{x^{1/2} + v/2},
$$

so that $\mu/(1 - \mu) = 2x^{1/2}/v$. Then

$$
-\mu (vx^{1/2} + x) + \frac{\mu^2 v^2}{4(1 - \mu)}
= -\mu (vx^{1/2} + x + v^2/4) + \frac{\mu v^2}{4(1 - \mu)}
= -\frac{x^{1/2}}{x^{1/2} + v/2} (x^{1/2} + v/2)^2 + \frac{2x^{1/2}v}{4} = -x
$$

and the result follows. \qed

Now we apply the Markov inequality

$$
\log \mathbb{P}(\gamma^\top B\gamma > p + 2vx^{1/2} + 2x) = \log \mathbb{P}((\gamma^\top B\gamma - p)/2 > vx^{1/2} + x)
\leq \inf_{\mu > 0} \left\{ -\mu (vx^{1/2} + x) + \log \mathbb{E} \exp\{\mu (\gamma^\top B\gamma - p)/2\} \right\}
\leq \inf_{\mu > 0} \left\{ -\mu (vx^{1/2} + x) + \frac{\mu^2 v^2}{4(1 - \mu)} \right\} \leq -x
$$

and the first assertion (D.1) follows. The second statement follows from the first one by $\text{tr}(B^2) \leq \|B\|_{\text{op}} \text{tr}(B) = \lambda p$.

Similarly for any $\mu > 0$

$$
\mathbb{P}(\gamma^\top B\gamma - p < -2\mu\sqrt{x}) \leq \exp(-\mu\sqrt{x}) \mathbb{E} \exp\left( -\frac{\mu}{2} (\gamma^\top B\gamma - p) \right).
$$

By (D.4)

$$
\log \mathbb{E} \exp\{ -\mu (\gamma^\top B\gamma - p)/2 \} = \frac{1}{2} \sum_{j=1}^{p} \{ \mu \lambda_j - \log(1 + \mu \lambda_j) \}
$$

and

$$
\frac{1}{2} \sum_{j=1}^{p} \{ \mu \lambda_j - \log(1 + \mu \lambda_j) \} = \frac{1}{2} \sum_{j=1}^{p} \sum_{k=2}^{\infty} \frac{(-\mu \lambda_j)^k}{k} \leq \sum_{j=1}^{p} \frac{(\mu \lambda_j)^2}{4} = \frac{\mu^2 v^2}{4}.
$$
Here the choice $\mu = 2\sqrt{x}/v$ yields (D.3).

One can put together the arguments used for obtaining the lower and the upper bound for getting a bound for a general quadratic form $\gamma^\top B\gamma$, where $B$ is symmetric but not necessarily positive.

Finally we apply this result to weighted sums of centered $\gamma_i^2$.

**Corollary D.4.** For any unit vector $u = (u_i) \in \mathbb{R}^n$ and standard normal r.v.'s $\gamma_i$, it holds with $\|u\|_\infty \overset{\text{def}}{=} \max_i |u_i|$

$$
\mathbb{P}\left( \left| \sum_{i=1}^n u_i (\gamma_i^2 - 1) \right| \geq 2x^{1/2} + 2\|u\|_\infty x \right) \leq 2e^{-x}.
$$

**Proof.** The statement follows directly from Theorem D.1. It suffices to notice $v^2 = \|u\|^2 = 1$.

As a special case, we present a bound for the chi-squared distribution corresponding to $B = I_p$. Then $\text{tr}(B) = p$, $\text{tr}(B^2) = p$ and $\lambda(B) = 1$.

**Corollary D.5.** Let $\gamma$ be a standard normal vector in $\mathbb{R}^n$. Then

$$
\begin{align*}
\mathbb{P}(\|\gamma\|^2 \geq p + 2\sqrt{p}x + 2x) &\leq e^{-x}, \\
\mathbb{P}(\|\gamma\| \geq \sqrt{p} + \sqrt{2}x) &\leq e^{-x}, \\
\mathbb{P}(\|\gamma\|^2 \leq p - 2\sqrt{p}x) &\leq e^{-x}.
\end{align*}
$$

The previous results are mainly stated for a standard Gaussian vector $\gamma \in \mathbb{R}^n$. Now we extend it to the case of a zero mean Gaussian vector $\xi$ with the $n \times n$ covariance matrix $\mathbb{V} = (\sigma_{ij})$ with $\lambda_{\text{max}}(\mathbb{V}) \leq \lambda^*$. Given a unit vector $u = (u_1, \ldots, u_n)^\top \in \mathbb{R}^n$, consider the quadratic form

$$
Q = \sum_{i=1}^n u_i \xi_i^2.
$$

We aim at bounding $Q - \mathbb{E}Q$. To apply the result of Theorem D.1 represent $Q$ as $\gamma^\top B\gamma$ with $B$ depending on $u$ and $\mathbb{V}$. More precisely, let $\xi = \mathbb{V}^{1/2}\gamma$ for a standard Gaussian vector $\gamma \in \mathbb{R}^n$. Then with $U = \text{diag}(u_1, \ldots, u_n)$, it holds

$$
S = \text{tr}(U\xi\xi^\top) = \text{tr}(U\mathbb{V}^{1/2}\gamma\gamma^\top\mathbb{V}^{1/2}) = \text{tr}(B\gamma\gamma^\top) = \gamma^\top B\gamma
$$

with $B = \mathbb{V}^{1/2}U\mathbb{V}^{1/2}$. Therefore, the bound $\|\mathbb{V}\|_{\text{op}} \leq \lambda^*$ implies

$$
\lambda = \lambda(B) = \|\mathbb{V}^{1/2}U\mathbb{V}^{1/2}\|_{\text{op}} \leq \lambda^* \|u\|_\infty ,
$$

$$
v^2 = \text{tr}(B^2) = \text{tr}(\mathbb{V}^{1/2}U\mathbb{V}U\mathbb{V}^{1/2}) \leq \lambda^* \text{tr}(U\mathbb{V}U) \leq \lambda^2 \|u\|^2 = \lambda^2.
$$
Now the general results of Theorem D.1 implies the result similar to Corollary D.4.

Corollary D.6. For any unit vector \( \mathbf{u} = (u_i) \in \mathbb{R}^n \), \( \|\mathbf{u}\| = 1 \), and normal zero mean vector \( \xi \sim N(0, \mathcal{V}) \) in \( \mathbb{R}^n \) with \( \|\mathcal{V}\|_{\text{op}} \leq \lambda^* \), it holds

\[
P \left( \left\| \sum_{i=1}^{n} u_i (\xi_i^2 - \mathbb{E}\xi_i^2) \right\| \geq 2\lambda^* x^{1/2} + 2\lambda^* \|\mathbf{u}\|_{\infty} x \right) \leq 2e^{-x}.
\]

It is worth noting that the identity \( \|\mathbf{u}\| = 1 \) implies \( \|\mathbf{u}\|_{\infty} \leq 1 \). Moreover, in typical situations, \( \|\mathbf{u}\|_{\infty} \asymp n^{-1/2} \), and the leading term in the bounds of Corollaries D.4 and D.6 is \( 2\lambda^* x^{1/2} \).

E Sums of random matrices

Here we present a number of deviation bounds for a sum of random matrices.

E.1 Matrix Bernstein inequality

This section collects some useful facts about deviation of stochastic matrices from their mean. We mainly use the arguments from the book Tropp (2015). The main step of the proof is the following Master bound.

Theorem E.1 (Master bound). Assume that \( \mathbf{S}_1, \ldots, \mathbf{S}_n \) are independent Hermitian matrices of the same size and \( \mathbf{Z} = \sum_{i=1}^{n} \mathbf{S}_i \). Then

\[
\mathbb{E}\lambda^+_{\max}(\mathbf{Z}) \leq \inf_{\theta > 0} \frac{1}{\theta} \log \text{tr} \exp \left( \sum_{i=1}^{n} \log \mathbb{E}e^{\theta \mathbf{S}_i} \right),
\]

\[
P\{\lambda^+_{\max}(\mathbf{Z}) \geq z\} \leq \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp \left( \sum_{i=1}^{n} \log \mathbb{E}e^{\theta \mathbf{S}_i} \right),
\]

where \( \lambda^+_{\max}(\mathbf{Z}) \) denotes the algebraically largest eigenvalue of \( \mathbf{Z} \).

For the proof see e.g. Tropp (2015).

The same result applied to \( -\mathbf{Z} \) yields the bound for the operator norm \( \|\mathbf{Z}\|_{\text{op}} \):

\[
P\{\|\mathbf{Z}\|_{\text{op}} \geq z\} \leq \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp \left( \sum_{i=1}^{n} \log \mathbb{E}e^{\theta \mathbf{S}_i} \right) + \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp \left( \sum_{i=1}^{n} \log \mathbb{E}e^{-\theta \mathbf{S}_i} \right). \tag{E.1}
\]
E.2 Matrix deviation bounds

The next result provides a deviation bound for a matrix-valued quadratic forms.

**Proposition E.2** (Deviation bound for matrix quadratic forms). Consider a $p \times n$ matrix $U$ such that

$$UU^\top = I_p.$$ 

Let the columns $\omega_1, \ldots, \omega_n \in \mathbb{R}^p$ of the matrix $U$ satisfy

$$\|\omega_i\| \leq \delta_n$$ \hspace{1cm} (E.2)

for a fixed constant $\delta_n$. For a random vector $\gamma = (\gamma_1, \ldots, \gamma_n)^\top$ with independent standard Gaussian components, define

$$Z \overset{\text{def}}{=} U \text{diag}\{\gamma \cdot \gamma - 1\}U^\top = \sum_{i=1}^n (\gamma_i^2 - 1)\omega_i\omega_i^\top.$$ 

Then with $x_p = x + \log(2p)$

$$\mathbb{P}(\|Z\|_{\text{op}} \geq 2\delta_n\sqrt{x_p} + 2\delta_n^2 x_p) \leq e^{-x}.$$ \hspace{1cm} (E.3)

**Proof.** From the Master bound (E.1)

$$\mathbb{P}(\|Z\|_{\text{op}} \geq z) \leq \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp\left(\sum_{i=1}^n \log \mathbb{E} \exp(\theta (\gamma_i^2 - 1)\omega_i\omega_i^\top)\right) + \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp\left(\sum_{i=1}^n \log \mathbb{E} \exp(\theta (-\gamma_i^2 + 1)\omega_i\omega_i^\top)\right).$$ \hspace{1cm} (E.4)

Now we use the following general fact:

**Lemma E.3.** If $\chi$ is a random variable and $\Pi$ is a projector in $\mathbb{R}^p$, then

$$\log \mathbb{E} \exp(\chi \Pi) = \log \left(\mathbb{E} e^{\chi}\right) \Pi.$$ \hspace{1cm} (E.5)

**Proof.** The result (E.5) can be easily obtained by applying twice the spectral mapping theorem.

This result yields, in particular, for any unit vector $\omega \in \mathbb{R}^p$

$$\log \mathbb{E} \exp(\chi \omega \omega^\top) = \log \left(\mathbb{E} e^{\chi}\right) \omega \omega^\top.$$
Moreover, for any vector $\omega \in \mathbb{R}^p$, the normalized product $\omega \omega^\top/\|\omega\|^2$ is a rank-one projector, and hence,

$$\log \mathbb{E} \exp(\chi \omega \omega^\top) = \log \left( \mathbb{E} e^{\chi\|\omega\|^2} \right) \frac{\omega \omega^\top}{\|\omega\|^2}.$$  

With $U_i \overset{\text{def}}{=} \omega_i \omega_i^\top/\|\omega_i\|^2$ and $\chi_i = \theta(\gamma_i^2 - 1)$, we derive

$$\log \mathbb{E} \exp\{\theta(\gamma_i^2 - 1)\omega_i \omega_i^\top\} = \log \mathbb{E} \exp\{\theta(\gamma_i^2 - 1)\|\omega_i\|^2\} U_i$$

$$= \log \left( \frac{\exp(-\|\omega_i\|^2\theta)}{\sqrt{1 - 2\|\omega_i\|^2\theta}} \right) U_i$$

$$= \left\{ -\|\omega_i\|^2\theta - \frac{1}{2} \log(1 - 2\theta\|\omega_i\|^2) \right\} U_i$$

and

$$\log \mathbb{E} \exp\{\theta(-\gamma_i^2 + 1)\omega_i \omega_i^\top\} = \log \mathbb{E} \exp\{\theta(-\gamma_i^2 + 1)\|\omega_i\|^2\} U_i$$

$$\leq -\|\omega_i\|^2\theta U_i$$

$$\leq \left\{ -\|\omega_i\|^2\theta - \frac{1}{2} \log(1 - 2\theta\|\omega_i\|^2) \right\} U_i.$$

Then it follows by (E.4)

$$\mathbb{P}(\|Z\|_{\text{op}} \geq z)$$

$$\leq 2 \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp\left\{ \sum_{i=1}^n \frac{\omega_i \omega_i^\top}{\|\omega_i\|^2} \left\{ -\|\omega_i\|^2\theta - \frac{1}{2} \log(1 - 2\theta\|\omega_i\|^2) \right\} \right\}. \tag{E.6}$$

Denote $\eta = (\eta_1, \ldots, \eta_n)^\top$, where

$$\eta_i = -\theta - \frac{\log(1 - 2\|\omega_i\|^2\theta)}{2\|\omega_i\|^2}.$$  

The use of (D.5) and (E.2) yields for $\theta < (2\delta_n^2)^{-1}$

$$\eta_i = \frac{1}{2}\|\omega_i\|^2 \left\{ 2\theta\|\omega_i\|^2 - \log(1 - 2\theta\|\omega_i\|^2) \right\}$$

$$\leq \frac{(2\theta\|\omega_i\|^2)^2}{4\|\omega_i\|^2(1 - 2\theta\delta_n^2)} \leq \frac{\theta^2\delta_n^2}{(1 - 2\theta\delta_n^2)}.$$  

Then by (E.6) and $UU^\top = I_p$ using $\mu = 2\theta\delta_n^2$

$$\mathbb{P}(\|Z\|_{\text{op}} \geq z) \leq 2 \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp\{U \text{diag}(\eta) U^\top\} \leq 2 \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp\{\|\eta\|_\infty I_p\}$$

$$\leq 2p \inf_{\mu > 0} \exp\left\{ -\theta z + \frac{\theta^2\delta_n^2}{1 - 2\theta\delta_n^2} \right\} = 2p \inf_{\mu > 0} \exp\left\{ -\mu z + \frac{\mu^2\delta_n^{-2}}{1 - \mu} \right\}.$$
Lemma D.3 helps to bound for $x_p = x + \log(2p)$ and $z = 2\delta_n x_p^{1/2} + 2\delta_n^2 x_p$ that

$$\inf_{\mu > 0} \exp \left\{-\mu \frac{z}{2\delta_n} + \frac{\mu^2 \delta_n^{-2}}{1 - \mu} \right\} = \inf_{\mu > 0} \left\{-\mu \left(\delta_n^{-1} x_p^{1/2} + x_p\right) + \frac{\mu^2 \delta_n^{-2}}{4(1 - \mu)} \right\} \leq -x_p.$$  

Therefore,

$$\mathbb{P}\left(\|Z\|_{\text{op}} \geq 2\delta_n \sqrt{x_p} + 2\delta_n^2 x_p\right) \leq 2pe^{-x} = e^{-x}$$

as required.  

**Proposition E.4** (Deviation bound for matrix Gaussian sums). Let vectors $\omega_1, \ldots, \omega_n$ in $\mathbb{R}^p$ satisfy

$$\|\omega_i\| \leq \delta_n$$

for a fixed constant $\delta_n$. Let $\gamma_i$ be independent standard Gaussian, $i = 1, \ldots, n$. Then for each vector $B = (b_1, \ldots, b_n)^\top \in \mathbb{R}^n$, the matrix $Z_1$ with

$$Z_1 \overset{\text{def}}{=} \sum_{i=1}^n \gamma_i b_i \omega_i \omega_i^\top$$

fulfills

$$\mathbb{P}\left(\|Z_1\|_{\text{op}} \geq \delta_n^2 \|B\| \sqrt{2x}\right) \leq 2e^{-x}.$$  

**Proof.** As $\gamma_i$ are i.i.d. standard normal and $\mathbb{E}e^{a\gamma_i} = e^{a^2/2}$ for $|a| < 1/2$, it follows from the Master inequality and Lemma E.3

$$\mathbb{P}\left(\|Z_1\|_{\text{op}} \geq z\right) \leq 2 \inf_{\theta > 0} e^{-\theta z} \text{tr} \exp \left\{\sum_{i=1}^n \log \mathbb{E} \exp(\theta \gamma_i b_i \omega_i \omega_i^\top)\right\}.$$

Moreover, as $\|\omega_i\| \leq \delta_n$ and $U_i = \omega_i \omega_i^\top / \|\omega_i\|^2$ is a rank-one projector with $\text{tr} U_i = 1$, it holds

$$\text{tr} \exp \left\{\frac{\theta^2}{2} \sum_{i=1}^n b_i^2 \|\omega_i\|^4 U_i\right\} \leq \exp \text{tr} \left(\frac{\theta^2 \delta_n^4}{2} \sum_{i=1}^n b_i^2 U_i\right) = \exp \frac{\theta^2 \delta_n^4 \|B\|^2}{2}.$$  

This implies for $z = \delta_n^2 \|B\| \sqrt{2x}$

$$\mathbb{P}\left(\|Z_1\|_{\text{op}} \geq z\right) \leq 2 \inf_{\theta > 0} \exp \left(-\theta z + \frac{1}{2} \theta^2 \delta_n^4 \|B\|^2\right) = 2e^{-x}$$

and the assertion follows.  

\[\square\]
E.3 Matrix valued quadratic forms

Let \( \xi = (\xi_1, \ldots, \xi_n)^\top \in \mathbb{R}^n \) be a Gaussian zero mean vector with the covariance matrix \( \mathbb{V} \) such that \( \|\mathbb{V}\|_{\text{op}} = \lambda_{\text{max}}(\mathbb{V}) \leq \lambda^* \). Let also \( \mathcal{U} \) be a \( p \times n \) matrix with columns \( \omega_1, \ldots, \omega_n \in \mathbb{R}^p \) such that

\[
\text{tr}(\mathcal{U}\mathcal{U}^\top) = \sum_{i=1}^{n} \|\omega_i\|^2 \leq q, \quad \max_{i} \|\omega_i\|^2 \leq \delta_n.
\]

(E.7)

A typical situation we have in mind is when

\[
\sum_{i=1}^{n} \omega_i\omega_i^\top = \mathbb{I}_p.
\]

Then (E.7) is satisfied with \( q = p \). Moreover, it also holds \( \text{tr}\{(\mathcal{U}\mathcal{U}^\top)^2\} = \text{tr}(\mathcal{U}\mathcal{U}^\top) = p \). Consider the \( p \times p \) random matrix \( \mathcal{B}_0 \) given by

\[
\mathcal{B}_0 \overset{\text{def}}{=} \sum_{i=1}^{n} \omega_i\omega_i^\top (\xi_i^2 - \mathbb{E}\xi_i^2).
\]

(E.8)

In the case of \( \mathbb{V} = \mathbb{I}_n \), Proposition E.2 provides a bound for the operator norm of \( \mathcal{B}_0 \). Below we extend this result to the case of a general matrix \( \mathbb{V} \) and establish similar bounds for quadratic forms of a non-centered vectors \( \xi + \mathcal{B} \). Also we evaluate the nuclear and Frobenius norms of this matrix. We begin with establishing a bound on the Frobenius norm of \( \mathcal{B}_0 \).

**Proposition E.5.** Let vectors \( \omega_i \in \mathbb{R}^p \) fulfill (E.7). Let also \( \xi \sim \mathcal{N}(0, \mathbb{V}) \) be a zero mean Gaussian vector \( \|\mathbb{V}\|_{\text{op}} \leq \lambda^* \). Then the random matrix \( \mathcal{B}_0 \) from (E.8) satisfies

\[
P\left( \text{tr}(\mathcal{B}_0^2) > 2\lambda^*\delta_n^2 q (x_n^{1/2} + \delta^* x_n) \right) \leq e^{-x}, \quad (E.9)
\]

where \( \delta^* \leq 1 \) and \( x_n = x + \log(n) \).

**Proof.** Denote \( \eta_i = \xi_i^2 - \mathbb{E}\xi_i^2 \) and \( c_{ij} = \omega_i^\top\omega_j \). Then

\[
\text{tr}(\mathcal{B}_0^2) = \sum_{i,j=1}^{n} \sum_{i=1}^{n} \eta_i \eta_j \text{tr}(\omega_i\omega_i^\top\omega_j\omega_j^\top) = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij}^2 \eta_i \eta_j.
\]

The \( n \times n \) matrix \( \mathbb{C} \overset{\text{def}}{=} (c_{ij}^2) \) is obviously symmetric positive. Therefore, one can represent it in the form \( \mathbb{C} = \mathbb{U}\mathbb{M}\mathbb{U}^\top \) for a diagonal matrix \( \mathbb{M} = \text{diag}(\mu_1, \ldots, \mu_n) \) and an orthonormal \( n \times n \) matrix \( \mathbb{U} = (\mathbf{u}_1, \ldots, \mathbf{u}_n) \) whose columns \( \mathbf{u}_k \) are orthonormal vectors in \( \mathbb{R}^n \). Therefore, for the vector \( \eta = (\eta_1, \ldots, \eta_n)^\top \),

\[
\text{tr}(\mathcal{B}_0^2) = \eta^\top \mathbb{C} \eta = \eta^\top \mathbb{U}\mathbb{M}\mathbb{U}^\top \eta = \sum_{k=1}^{n} \mu_k |\mathbf{u}_k^\top \eta|^2.
\]

(E.10)
Further, one can bound each $u_k^T \eta$ by the result of Corollary D.6: for any $x_n > 0$
\[
\mathbb{P}\left(\left|u_k^T \eta\right| > 2\lambda^* \left(x_n^{1/2} + \|u_k\|_\infty x_n\right)\right) \leq e^{-x_n}.
\]
The choice $x_n = x + \log(n)$ and (E.10) imply
\[
\mathbb{P}\left(\text{tr}(B_0^2) > \sum_{k=1}^n 2\lambda^* \mu_k \left(x_n^{1/2} + \|u_k\|_\infty x_n\right)\right) \leq e^{-x}.
\]
Also by construction and (E.7)
\[
\sum_{k=1}^n \mu_k = \text{tr}(C) = \sum_{i=1}^n c_{ii}^2 = \sum_{i=1}^n \|\omega_i\|^4 \leq \delta_n^2 \text{tr}\left(\sum_{i=1}^n \omega_i \omega_i^T\right) = \delta_n^2 q.
\]
The result (E.9) uses a very rough bound $\|u_k\|_\infty \leq \delta^*$ for some constant $\delta^* \leq 1$. In typical situation one can refine it to $\|u_k\|_\infty \leq C \delta_n$.

Now we consider a slightly more general situation with a bias component. Given a bias vector $B$ in $\mathbb{R}^n$, a $p \times n$ matrix $U$, and a stochastic Gaussian zero mean vector $\xi$, define a random $p \times p$ matrix $B_1 \overset{\text{def}}{=} U \text{diag}\left\{(\xi + B) \cdot (\xi + B) - \xi \cdot \xi\right\} U^T$.

The next result bounds the values $\text{tr}(B_1)$ and $\text{tr}(B_1^2)$.

**Proposition E.6.** Suppose that a Gaussian vector $\xi \sim \mathcal{N}(0, V)$ satisfies
\[
\delta_1 \overset{\text{def}}{=} \|V - I_n\|_{\text{op}}, \tag{E.11}
\]
Let also $UU^T \leq I_p$ and the vectors $\omega_i$ - columns of $U$ - satisfy for some $q_2 \leq q$
\[
\text{tr}(UU^T) = \sum_{i=1}^n \|\omega_i\|^2 \leq q, \tag{E.12}
\]
\[
\text{tr}\left((UU^T)^2\right) = \sum_{i,j=1}^n \|\omega_i^T \omega_j\|^2 \leq q_2,
\]
\[
\max_i \|\omega_i\| \leq \delta_n.
\]
Then on a random set $\Omega_{10}(x)$ with $\mathbb{P}(\Omega_{10}(x)) \geq 1 - 2e^{-x}$, it holds
\[
\|B_1\|_{\text{op}} \leq \|B\|_\infty^2 + \delta_n^2 \|B\|\sqrt{2x} \tag{E.13}
\]
and on a random set $\Omega_{11}(x)$ with $\mathbb{P}(\Omega_{11}(x)) \geq 1 - e^{-x}$, it holds
\[
\left|\text{tr}(B_1)\right| \leq q \|B\|_\infty^2 + 4 x^{1/2} \delta_n^2 \|B\|. \tag{E.14}
\]
Further, $\|B_1\|_{Fr} = \sqrt{\text{tr}(B_1^2)}$ fulfills on a random set $\Omega_{12}(x)$ with $\mathbb{P}(\Omega_{12}(x)) \geq 1 - e^{-x}$

$$\|B_1\|_{Fr} \leq \Delta_1(x),$$

$$\Delta_1(x) \overset{\text{def}}{=} \sqrt{\|B\|_{\infty}^2 q_2 + 4\delta_n^2 \|B\| (1 + \sqrt{x})}.$$

**Proof.** We use the representation

$$B_1 = U \text{diag}\left\{(\xi + B) \cdot (\xi + B)\right\} U^\top - U \text{diag}\{\xi \cdot \xi\} U^\top = U \text{diag}\{B \cdot B\} U^\top + 2 U \text{diag}\{\xi \cdot B\} U^\top.$$

It obviously holds with $\|B_1\|_{Fr} \overset{\text{def}}{=} \sqrt{\text{tr}(B_1^2)}$

$$|\text{tr}(B_1)| \leq |\text{tr}(B_{11})| + |\text{tr}(B_{12})|,$$

$$\|B_1\|_{Fr} \leq \|B_{11}\|_{Fr} + \|B_{12}\|_{Fr}.$$  \hspace{1cm} (E.15)

We proceed with each $B_{1m}$ for $m = 1, 2$ separately starting from $B_{11}$.

**Bounds for $B_{11}$:** The bias term $B_{11}$ can be estimated as follows:

$$\|B_{11}\|_{op} = \left\| \sum_{i=1}^n \omega_i \omega_i^\top b_i^2 \right\|_{op} \leq \|B\|_{\infty}^2 \|UU^\top\|_{op} \leq \|B\|_{\infty}^2,$$

$$\text{tr}(B_{11}) = \text{tr}\left(\sum_{i=1}^n \omega_i \omega_i^\top b_i^2\right) \leq \|B\|_{\infty}^2 \text{tr}(UU^\top) \leq q \|B\|_{\infty}^2,$$ \hspace{1cm} (E.16)

$$\text{tr}(B_{11}^2) = \text{tr}\left(\sum_{i=1}^n \omega_i \omega_i^\top b_i^2\right)^2 \leq \|B\|_{\infty}^4 \text{tr}\{(UU^\top)^2\} \leq q_2 \|B\|_{\infty}^4.$$

Another way of bounding the value $\text{tr}(B_{11}^2)$ is based on the condition $\|\omega_i\| \leq \delta_n$. Then for any unit vector $\gamma \in \mathbb{R}^p$, it holds $|\gamma^\top \omega_i| \leq \delta_n$ and

$$\gamma^\top B_{11} \gamma = \sum_{i=1}^n |\omega_i^\top \gamma|^2 b_i^2 \leq \delta_n^2 \sum_{i=1}^n b_i^2 = \delta_n^2 \|B\|^2.$$

Therefore, $\|B_{11}\|_{op} \leq \delta_n^2 \|B\|^2$ and hence,

$$\text{tr}(B_{11}^2) \leq (\delta_n^2 \|B\|^2)^p = \delta_n^4 \|B\|^4 p.$$

Note, however, that the bound (E.16) is typically more accurate: the value $\delta_n^2$ is of order $q/n$ and $\|B\|^2 \asymp n \|B\|_{\infty}^2$, so that $\delta_n^4 \|B\|^4 p \gg q_2 \|B\|_{\infty}^4$ for $p$ large.
Bounds for $\mathcal{B}_{12}$: Proposition E.4 provides a bound for $\mathcal{B}_{12}$ in the operator norm for standard Gaussian $\xi$:

$$P\left(\|\mathcal{B}_{12}\|_{op} \geq \delta_n^2 \|\mathbf{B}\|\sqrt{2x}\right) \leq 2e^{-x}.$$ 

Now we bound $\text{tr}(\mathcal{B}_{12})$ and $\text{tr}(\mathcal{B}_{12}^2)$. By definition,

$$\text{tr}(\mathcal{B}_{12}) = 2 \text{tr}\left(\sum_{i=1}^{n} \mathbf{w}_i \mathbf{w}_i^\top \xi_i b_i\right) = 2 \sum_{i=1}^{n} \|\mathbf{w}_i\|^2 \xi_i b_i = 2\mathbf{u}^\top \xi,$$

where $\mathbf{u}$ is the vector in $\mathbb{R}^n$ with the entries $u_i = \|\mathbf{w}_i\|^2 b_i$. As $\text{Var}(\xi) = \mathbf{V}$ with $\|\mathbf{V}\|_{op} \leq 2$, $\mathbf{u}^\top \xi$ is a Gaussian zero mean random variable whose variance satisfies

$$\text{Var}(\mathbf{u}^\top \xi) \leq \mathbf{u}^\top \mathbf{V} \mathbf{u} \leq 2 \|\mathbf{u}\|^2 = 2 \sum_{i=1}^{n} \|\mathbf{w}_i\|^2 b_i^2 \leq 2\delta_n^4 \|\mathbf{B}\|^2.$$ 

Here we have used (E.11) and $\|\mathbf{w}_i\| \leq \delta_n$. Therefore, on a random set $\Omega_{12}(x)$ with $P(\Omega_{12}(x)) \geq 1 - e^{-x}$,

$$|\text{tr}(\mathcal{B}_{12})| \leq 2\sqrt{2} \delta_n^2 \|\mathbf{B}\| z_1(x) \leq 4x^{1/2} \delta_n^2 \|\mathbf{B}\|,$$

where $z_1(x) \leq \sqrt{2x}$ is given by $P(|\gamma| > z_1(x)) = e^{-x}$ for a standard normal $\gamma$.

It remains to bound $\text{tr}(\mathcal{B}_{12}^2)$. Because of cross-dependence of the $\xi_i$’s, we cannot directly apply the result of Proposition E.4. Instead we use the following representation:

$$\text{tr}(\mathcal{B}_{12}^2) = 4 \sum_{i,j=1}^{n} (\mathbf{w}_i^\top \mathbf{w}_j)^2 b_i b_j \xi_i \xi_j.$$ 

Denote by $\mathbf{C}_1$ the $n \times n$ matrix with the entries $(\mathbf{w}_i^\top \mathbf{w}_j)^2 b_i b_j$ for $i, j = 1, \ldots, n$. The use of $\xi = \mathbf{V}^{1/2} \gamma$ with $\mathbf{V} = \text{Var}(\xi)$ and a standard normal $\gamma \in \mathbb{R}^n$ yields

$$\text{tr}(\mathcal{B}_{12}^2) = 4\mathbf{\xi}^\top \mathbf{C}_1 \mathbf{\xi} = 4\gamma^\top \mathbf{V}^{1/2} \mathbf{C}_1 \mathbf{V}^{1/2} \gamma = 4\gamma^\top \mathbf{C}_2 \gamma,$$

where $\mathbf{C}_2 = \mathbf{V}^{1/2} \mathbf{C}_1 \mathbf{V}^{1/2}$. Now the bound of Proposition D.1 on Gaussian quadratic forms is well applicable. It holds

$$p(\mathbf{C}_2) = \text{tr}(\mathbf{C}_2) \leq 2 \text{tr}(\mathbf{C}_1) = 2 \sum_{i=1}^{n} \|\mathbf{w}_i\|^4 b_i^2 \leq 2\delta_n^4 \|\mathbf{B}\|^2.$$ 

Similarly for any unit vector $\mathbf{u} \in \mathbb{R}^n$, it holds by $|\mathbf{w}_i^\top \mathbf{w}_j| \leq \delta_n^2$

$$\mathbf{u}^\top \mathbf{C}_1 \mathbf{u} = \sum_{i,j=1}^{n} u_i u_j b_i b_j (\mathbf{w}_i^\top \mathbf{w}_j)^2 \leq \delta_n^4 \left(\sum_{i=1}^{n} u_i b_i\right)^2 \leq \delta_n^4 \|\mathbf{u}\|^2 \|\mathbf{B}\|^2 = \delta_n^4 \|\mathbf{B}\|^2.$$
yielding \( \lambda_{\max}(C_1) \leq \delta_n^4 \| B \|_2^2 \) and
\[
\lambda(C_2) \overset{\text{def}}{=} \lambda_{\max}(C_2) \leq 2\delta_n^4 \| B \|_2^2.
\]
Proposition D.1 implies on a random set of probability at least \( 1 - e^{-x} \)
\[
\sqrt{\text{tr}(\mathcal{B}_1^2)} = 2\sqrt{\gamma^2 C_2 \gamma}
\]
\[
\leq 2\sqrt{p(C_2)} + 2\sqrt{2\lambda(C_2)x}
\]
\[
= 2\sqrt{2} \delta_n^2 \| B \|_2 (1 + \sqrt{x})
\]
\[
\leq 4 \delta_n^2 \| B \|_2 (1 + \sqrt{x}).
\]
Putting all bounds together yields by (E.15) the statements of the proposition.

Now we evaluate the effect of presmoothing in the stochastic component. Let \( \xi \) be normal zero mean vector in \( \mathbb{R}^p \) with a covariance matrix \( V \) satisfying (E.11). The goal is to bound the values \( \text{tr}(B_2) \) and \( \text{tr}(B_2^2) \) for the difference
\[
B_2 \overset{\text{def}}{=} \mathcal{U} \text{diag}(\xi \cdot \xi - \mathbb{E}(\xi \cdot \xi)) \mathcal{U}^\top.
\]

**Proposition E.7.** Suppose that \( \xi \sim N(0, V) \) with \( V \) satisfying (E.11). Let also \( \mathcal{V} \mathcal{U}^\top \leq I_p \) and the vectors \( \omega_i \) - columns of \( \mathcal{U} \) - satisfy (E.12) for some \( q_2 \leq q \). Then on a random set \( \Omega_{22}(x) \) with \( \mathbb{P}(\Omega_{22}(x)) \geq 1 - e^{-x} \), it holds for \( \| B_2 \|_F = \sqrt{\text{tr}(B_2^2)} \)
\[
\| B_2 \|_F \leq \Delta_2(x) \overset{\text{def}}{=} 2\sqrt{x} q \delta_n^2.
\]
Moreover, on a random set \( \Omega_{21}(x) \) with \( \mathbb{P}(\Omega_{21}(x)) \geq 1 - 2e^{-x} \), it holds
\[
|\text{tr}(B_2)| \leq 4\sqrt{x} q \delta_n^2 + 4\sqrt{x} \delta_n^2.
\]

**Proof.** By (E.11), the covariance matrix \( V = \text{Var}(\xi) \) fulfills
\[
\| V \|_{\text{op}} \leq 1 + \delta_1 \leq 2.
\]
Now, by Proposition E.5, for \( x_n = x + \log(n) \) and \( \delta^* \leq 1 \), it holds on a random set \( \Omega_{22}'(x) \) with \( \mathbb{P}(\Omega_{22}'(x)) \geq 1 - e^{-x} \)
\[
\text{tr}(B_2^2) \leq 2(1 + \delta_1) \delta_n^2 q (x_n^{1/2} + \delta^* x_n).
\]
Here \( \delta^* \leq 1 \), usually \( \delta^* \ll 1 \), and \( \delta_1 \leq 1 \), so we simplify the bound to
\[
\text{tr}(B_2^2) \leq 4 x_n q \delta_n^2.
\]
Now we bound the trace $\text{tr}(B_2)$. By definition, it holds for columns $\omega_i \in \mathbb{R}^q$ of $U$

$$\text{tr}(B_2) = \sum_{i=1}^{n} \text{tr}(\omega_i \omega_i^\top) (\xi_i^2 - \mathbb{E}\xi_i^2) = \sum_{i=1}^{n} \|\omega_i\|^2 (\xi_i^2 - \mathbb{E}\xi_i^2),$$

and by Corollary D.6, it holds on a random set $\Omega_{21}(x)$ with $P(\Omega_{21}(x)) \geq 1 - 2e^{-x}$

$$|\text{tr}(B_2)| \leq 4x^{1/2} \left( \sum_{i=1}^{n} \|\omega_i\|^4 \right)^{1/2} + 4x \max_i \|\omega_i\|^2.$$

This implies in view of $\|\omega_i\| \leq \delta_n$ and (E.12)

$$\sum_{i=1}^{n} \|\omega_i\|^4 \leq \max_i \|\omega_i\|^2 \sum_{i=1}^{n} \|\omega_i\|^2 \leq q \delta_n^2.$$

Therefore, it holds on $\Omega_{21}(x)$

$$|\text{tr}(B_2)| \leq 4 \sqrt{x} q \delta_n^2 + 4 x \delta_n^2$$

as required.

Finally we bound the deterministic term

$$B_3 \overset{\text{def}}{=} U \text{diag}\{ \mathbb{E}(\xi \cdot \xi) - I_n \} U^\top.$$  \hspace{1cm} (E.18)

**Proposition E.8.** Suppose that $\xi \sim \mathcal{N}(0, \Sigma)$ with

$$\delta_\varepsilon \overset{\text{def}}{=} \max_i |\mathbb{E}\xi_i^2 - 1|.$$

Let also $UU^\top \leq I_p$ and the vectors $\omega_i$ - columns of $U$ - satisfy (E.12) for some $q_2 \leq q$. Then it holds for the matrix $B_3$ from (E.18)

$$|\text{tr}(B_3)| \leq \delta_\varepsilon q,$$

$$\text{tr}(B_3^2) \leq \Delta_3(x) \overset{\text{def}}{=} \delta_\varepsilon^2 q_2.$$

**Proof.** By direct calculus, it holds in view of (E.12) and $|\mathbb{E}\xi_i^2 - 1| \leq \delta_\varepsilon$

$$\text{tr}(B_3^2) = \text{tr}\left( \sum_{i=1}^{n} \omega_i \omega_i^\top (\mathbb{E}\xi_i^2 - 1) \right)^2 \leq \delta_\varepsilon^2 \text{tr}\left( (UU^\top) \right)^2 \leq \delta_\varepsilon^2 q_2;$$

Further,

$$|\text{tr}(B_3)| \leq \text{tr}\left( \sum_{i=1}^{n} \omega_i \omega_i^\top |\mathbb{E}\xi_i^2 - 1| \right) \leq \delta_\varepsilon \text{tr}(UU^\top) \leq \delta_\varepsilon q.$$

This yields the assertion. \hfill \Box
Now we present a bound in the operator norm of the matrix $B$ with

$$B \overset{\text{def}}{=} U \operatorname{diag}\{(\xi + B) \cdot (\xi + B) - I_n\}U^T.$$

(E.20)

**Proposition E.9.** Assume the conditions of Proposition E.6, and let the rows $\Upsilon_i^T$ of $\Upsilon = \Sigma^{-1/2} II \Sigma^{1/2}$ satisfies $\|\Upsilon_i\| \leq \delta_n$. Then on a random set $\Omega_{\text{op}}(x)$ with $\mathcal{P}(\Omega_{\text{op}}(x)) \geq 1 - 6e^{-x}$, it holds with $x_n = x + \log(n)$ and $x_p = x + 2 \log(p)$ for $B$ from (E.20)

$$\|B\|_{\text{op}} \leq \Delta_{\text{op}}(x),$$

$$\Delta_{\text{op}}(x) \overset{\text{def}}{=} \|B\|_\infty^2 + \delta_n^2 \|B\| \sqrt{2x} + 2\delta_n x_p^{1/2} + 2\delta_n^2 x_p + 2\delta_n x_n + \delta_n^2 x_n.$$

**Proof.** We use the following decomposition:

$$B = U \operatorname{diag}\{(\xi + B) \cdot (\xi + B) - \xi \cdot \xi\}U^T \overset{\text{def}}{=} B_1$$

$$+ U \operatorname{diag}\{\xi \cdot \xi - \gamma \cdot \gamma\}U^T \overset{\text{def}}{=} B_4$$

$$+ U \operatorname{diag}\{\gamma \cdot \gamma - I_n\}U^T \overset{\text{def}}{=} B_5$$

Here $\gamma \overset{\text{def}}{=} \Sigma^{-1/2}\epsilon$ is a standard Gaussian vector. Obviously

$$\|B\|_{\text{op}} \leq \|B_1\|_{\text{op}} + \|B_4\|_{\text{op}} + \|B_5\|_{\text{op}}.$$

The value $\|B_1\|_{\text{op}}$ is already evaluated in (E.13) of Proposition E.6:

$$\|B_1\|_{\text{op}} \leq \|B\|_\infty^2 + \delta_n^2 \|B\| \sqrt{2x}$$

on a random set $\Omega_{10}(x)$ with $\mathcal{P}(\Omega_{10}(x)) \geq 1 - 2e^{-x}$. The matrix $B_5$ can be bounded by a version of matrix Bernstein inequality (E.3) in Proposition E.2: one a set $\Omega_5(x)$ with $\mathcal{P}(\Omega_5(x)) \geq 1 - 2e^{-x}$

$$\|B_5\|_{\text{op}} \leq 2\delta_n \sqrt{x_p} + 2\delta_n^2 x_p.$$

It remains to bound the value $\|B_4\|_{\text{op}}$. By definition, with $\Upsilon = \Sigma^{-1/2} II \Sigma^{1/2}

$$\xi = \Sigma^{-1/2}(\epsilon - II \epsilon) = \gamma - \Upsilon \gamma.$$

This obviously implies

$$\xi \cdot \xi - \gamma \cdot \gamma = (\Upsilon \gamma) \cdot (\Upsilon \gamma) - 2(\Upsilon \gamma) \cdot \gamma$$

and

$$\|B_4\|_{\text{op}} \leq \|U \operatorname{diag}\{(\Upsilon \gamma) \cdot (\Upsilon \gamma)\}U^T\|_{\text{op}} + 2\|U \operatorname{diag}\{(\Upsilon \gamma) \cdot \gamma\}U^T\|_{\text{op}}$$
The condition $UU^T \leq I_p$ helps to bound

$$
\|U \text{diag}\{(R\gamma) \cdot (R\gamma)\}U^T\|_{op} \leq \|R\gamma\|_\infty^2 \|UU^T\|_{op} \leq \|R\gamma\|_\infty^2.
$$

Similarly

$$
\|U \text{diag}\{(R\gamma) \cdot \gamma\}U^T\|_{op} \leq \|R\gamma\|_\infty \|\gamma\|_\infty \|UU^T\|_{op} \leq \|R\gamma\|_\infty \|\gamma\|_\infty.
$$

It is well known that the sup-norm of a standard Gaussian vector $\gamma$ can be bounded as

$$
\|\gamma\|_\infty \leq \sqrt{2x_n}
$$

with $x_n = x + \log(n)$ on a set of probability $1 - e^{-x}$. Further, if each row $Y_i^T$ of $Y$ satisfies $\|Y_i\| \leq \delta_n$, then the scalar product $Y_i^T \gamma$ is a normal zero mean r.v. with the variance

$$
\text{Var}(Y_i^T \gamma) = \|Y_i\|^2 \leq \delta_n^2
$$

and

$$
P(|Y_i^T \gamma| > \delta_n z_1(x)) \leq e^{-x}
$$

with $z_1(x) \leq \sqrt{2x}$ yielding

$$
P(\|R\gamma\|_\infty > \delta_n \sqrt{2x_n}) \leq e^{-x}.
$$

Summing together results in the bound

$$
\|B_4\|_{op} \leq 2\delta_n x_n + \delta_n^2 x_n
$$

on a set $\Omega_4(x)$ with $P(\Omega_4(x)) \geq 1 - 2e^{-x}$.

F Gaussian comparison via KL-divergence and Pinsker’s inequality

Suppose that two $p$-dimensional zero mean Gaussian vectors $\xi \sim N(0, S)$ and $\xi^b \sim N(0, S^b)$ are given. Let also $T$ map $R^p$ to $R^M$ and $X = T(\xi)$ and $Y = T(\xi^b)$. We aim to bound the distance between distributions of $X$ and $Y$ under the conditions

$$
\|S^{-1/2}S^bS^{-1/2} - I_p\|_{op} \leq \epsilon \leq 1/2,
$$

$$
\text{tr}(S^{-1/2}S^bS^{-1/2} - I_p)^2 \leq \Delta^2
$$

(F.1)

for some $\epsilon \leq 1/2$ and $\Delta \geq 0$. The next lemma bounds from above the Kullback-Leibler divergence between two normal distributions.
Lemma F.1. Let $P_0 = N(b, S)$ and $P_1 = N(b^\prime, S^\prime)$ for some non-degenerated matrices $S$ and $S^\prime$. If

$$\|S^{-1/2}S^\prime S^{-1/2} - I_p\|_{\text{op}} \leq 1/2,$$

$$\text{tr}\left\{ (S^{-1/2}S^\prime S^{-1/2} - I_p)^2 \right\} \leq \Delta^2,$$

then

$$\mathcal{K}(P_0, P_1) = -2\mathbb{E}_0 \log \frac{dP_1}{dP_0} \leq \frac{\Delta^2}{2} + \frac{1}{2}(b - b^\prime)^\top S^\prime(b - b^\prime).$$

For any measurable set $A \subset \mathbb{R}^p$, it holds

$$\left| P_0(A) - P_1(A) \right| \leq \sqrt{\mathcal{K}(P_0, P_1)}/2.$$

**Proof.** The change of variables $u = S^{-1/2}(x-b)$ reduces the general case to the situation where $P_0$ is standard normal in $\mathbb{R}^p$ while $P_1 = N(\beta, B)$ with $\beta = S^{1/2}(b^\prime - b)$ and $B \overset{\text{def}}{=} S^{-1/2}S^\prime S^{-1/2}$

$$2 \log \frac{dP_1}{dP_0}(\gamma) = \log \det(B) - (\gamma - \beta)^\top B(\gamma - \beta) + \|\gamma\|^2$$

with $\gamma$ standard normal and

$$2\mathcal{K}(P_0, P_1) = -2\mathbb{E}_0 \log \frac{dP_1}{dP_0} = -\log \det(B) + \text{tr}(B - I_p) + \beta^\top B\beta.$$

Let $a_j$ be the $j$th eigenvalue of $B - I_p$. The condition $\|B - I_p\|_{\text{op}} \leq 1/2$ yields $|a_j| \leq 1/2$ and

$$2\mathcal{K}(P_0, P_1) = \beta^\top B\beta + \sum_{j=1}^p \left\{ a_j - \log(1 + a_j) \right\}$$

$$\leq \beta^\top B\beta + \sum_{j=1}^p a_j^2$$

$$\leq \beta^\top B\beta + \text{tr}(B - I_p)^2 \leq \beta^\top B\beta + \Delta^2.$$

This implies by Pinsker’s inequality

$$\sup_A |P_0(A) - P_1(A)| \leq \sqrt{\frac{1}{2} \mathcal{K}(P_0, P_1)} \leq \frac{1}{2} \sqrt{\Delta^2 + \beta^\top B\beta}$$

as required. \hfill \Box

Notice that the operator norm bound

$$\|S^{-1/2}S^\prime S^{-1/2} - I_p\|_{\text{op}} \leq \epsilon$$

(F.2)
implies for $B = S^{-1/2}S^bS^{-1/2}$

$$\text{tr}(B - I_p)^2 \leq p\epsilon^2, \quad \beta^\top B\beta \leq (1 + \epsilon)\|\beta\|^2.$$  

**Corollary F.2.** Let $\mathcal{P}_0 = \mathcal{N}(b, S)$ and $\mathcal{P}_1 = \mathcal{N}(b^b, S^b)$ for some non-degenerated matrices $S$ and $S^b$ satisfying (F.2). Then

$$\sup_A |\mathcal{P}_0(A) - \mathcal{P}_1(A)| \leq \frac{1}{2}\sqrt{p\epsilon^2 + (1 + \epsilon)\|\beta\|^2}$$

For the special case with $\beta \equiv 0$, we bound for any Borel set $A \subset \mathbb{R}^M$

$$|\mathcal{P}(T(\xi) \in A) - \mathcal{P}(T(\xi^b) \in A)| \leq \Delta/2.$$  

We state a separate corollary for the distribution of the maximum.

**Corollary F.3.** Let two $p$-dimensional zero mean Gaussian vectors $\xi \sim \mathcal{N}(0, S)$ and $\xi^b \sim \mathcal{N}(0, S^b)$ be given, and (F.1) holds. Then for any mapping $T: \mathbb{R}^p \to \mathbb{R}^M$ and any set of values $(q_\eta)$, the random vectors $X = T(\xi)$ and $Y = T(\xi^b)$ fulfill

$$|\mathcal{P}(\max_\eta X_\eta - q_\eta > 0) - \mathcal{P}(\max_\eta Y_\eta - q_\eta > 0)| \leq \Delta/2.$$  

**Proof.** We simply apply the result of the lemma to the set $A = \{x \in \mathbb{R}^p: T(x) \leq z\}$.  

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