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Estimating linear and quadratic forms via indirect observations

ANATOLI JUDITSKY[1] and ARKADI NEMIROVSKI[2]

[1] *LJK, Université Grenoble Alpes, 700 Avenue Centrale 38401 Domaine Universitaire de Saint-Martin-d'Hères, France. E-mail: anatoli.juditsky@univ-grenoble-alpes.fr*
[2] *Georgia Institute of Technology, Atlanta, GA 30332, USA. E-mail: nemirovs@isye.gatech.edu*

In this paper, we further develop the approach, originating in Juditsky and Nemirovski (*Ann. Statist.* **37** (2009) 2278–2300), to "computation-friendly" statistical estimation via Convex Programming.Our focus is on estimating a linear or quadratic form of an unknown "signal," known to belong to a given convex compact set, via noisy indirect observations of the signal. Classical theoretical results on the subject deal with precisely stated statistical models and aim at designing statistical inferences and quantifying their performance in a closed analytic form. In contrast to this traditional (highly instructive) descriptive framework, the approach we promote here can be qualified as operational – the estimation routines and their risks are not available "in a closed form," but are yielded by an efficient computation. All we know in advance is that under favorable circumstances the risk of the resulting estimate, whether high or low, is provably near-optimal under the circumstances. As a compensation for the lack of "explanatory power," this approach is applicable to a much wider family of observation schemes than those where "closed form descriptive analysis" is possible.

We discuss applications of this approach to classical problems of estimating linear forms of parameters of sub-Gaussian distribution and quadratic forms of parameters of Gaussian and discrete distributions. The performance of the constructed estimates is illustrated by computation experiments in which we compare the risks of the constructed estimates with (numerical) lower bounds for corresponding minimax risks for randomly sampled estimation problems.

Keywords: linear and quadratic functional estimation; linear estimation; statistical linear inverse problems

1. Introduction

In its most general form, the problem we are interested in this paper is as follows:

Given are:

- (nonempty convex compact) *signal set* $\mathcal{X} \subset \mathbf{R}^n$ and a (complete separable metric) *observation space* Ω
- a mapping $x \mapsto \mathcal{P}_x$ associating with *signal* $x \in \mathcal{X}$ a family of $\mathcal{P}_x$ of Borel probability distributions on Ω
- (linear or quadratic) function $G(x)$ on the signal set $\mathcal{X}$

Given *K-repeated observation* – a collection $\omega^K = (\omega_1, \dots, \omega_K)$ of i.i.d. random variables $\omega_k \sim P$ with probability distribution $P \in \mathcal{P}_x$ for some *unknown* $x \in \mathcal{X}$, we want to recover $G(x)$.
Note that we make no assumptions on how "the nature" (or an adversary) selects in $\mathcal{P}_x$ the probability distribution P of individual observation.

In this problem, a candidate estimate is a (whatever) Borel function $\omega^K \mapsto \widehat{G}(\omega^K) \in \mathbf{R}$; we quantify performance of this estimate by its ϵ*-risk*

$$\mathrm{Risk}_\epsilon\big(\widehat{G}(\cdot)|\mathcal{X}\big) = \inf\big\{\rho : \mathrm{Prob}_{\omega^K\sim P\times\cdots\times P}\big\{\big|\widehat{G}(\omega) - G(x)\big| > \rho\big\} \le \epsilon\ \forall(x \in \mathcal{X}, P \in \mathcal{P}_x)\big\} \quad (1.1)$$

– the worst, over signals $x \in \mathcal{X}$ and selections $P \in \mathcal{P}_x$, half-width of $(1-\epsilon)$-confidence interval associated with the estimate. Here $\epsilon \in (0, 1)$ is a once for ever fixed reliability tolerance.

To give an impression of our approach and results, consider the *sub-Gaussian* case of the above problem where $\mathcal{X}$ is a convex compact set in some $\mathbf{R}^n$, $G(x)$ is a given affine function, $\Omega = \mathbf{R}^m$, and $\mathcal{P}_x$, $x \in \mathcal{X}$, is comprised of all sub-Gaussian distributions with parameters affinely parameterized by x:

$$\mathcal{P}_x = \left\{P : \mathbf{E}_{\omega\sim P}\{\mathrm{e}^{f^T\omega}\} \le f^T\theta(x) + \frac{1}{2}f^T M(x) f\ \forall f \in \mathbf{R}^m\right\},$$

where $\theta(x)$, $M(x)$ are given affine in x mappings taking values in $\mathbf{R}^m$ and in the space $\mathbf{S}^m$ of symmetric $m \times m$ matrices, respectively, and such that $M(x)$ is positive semidefinite whenever $x \in \mathcal{X}$. Our related constructions and results can be outlined as follows:

- The estimate $\widehat{G}(\omega^K)$ we build is of the form $\widehat{G}(\omega^K) = \sum_{k=1}^K \widetilde{G}(\omega_k)$ stemming from *affine* function $\widetilde{G}(\omega)$; the coefficients of this function, same as an (upper bound on) the ϵ-risk of the estimate stem from an optimal solution to an explicit convex optimization problem and thus can be specified in a computationally efficient fashion.
- Under mild structural assumptions on the affine mapping $x \mapsto (\theta, \Theta)$ the resulting estimate is provably near-optimal in the minimax sense (see Section 4 for details). The latter statement is an extension of the fundamental result of Donoho [11] on near-optimality of affine recovery of a linear form of signal in Gaussian observation scheme $\omega \sim \mathcal{N}(\theta(x), \Theta)$.

This paper contributes to a long line of research on estimating linear (see, e.g., Levit [40], Ibragimov and Khas'minskii [25], Efromovich and Low [17], Lepski and Spokoiny [38], Klemela and Tsybakov [32], Juditsky and Nemirovski [27], Butucea and Comte [7] and references therein) and quadratic (Hasminskii and Ibragimov [22], Ibragimov, Nemirovskii and Khas'minskii [26], Bickel and Ritov [1], Fan [18], Donoho and Nussbaum [15], Birgé and Massart [6], Efromovich and Low [16], Laurent [33], Gayraud and Tribouley [19], Huang and Fan [24], Laurent and Massart [35], Laurent [34], Klemelä [31], Butucea and Meziani [8] among others) functionals of parameters of probability distributions via observations drawn from these distributions. In the majority of cited papers, the objective is to provide "closed analytical form" lower risk bounds for problems at hand and upper risk bounds for the proposed estimates, in good cases matching the lower bounds. This paradigm can be referred to as "descriptive;" it relies upon analytical risk analysis and estimate design and possesses strong explanation power. It, however, imposes severe restrictions on the structure of the statistical model, restrictions making the estimation problem amenable to complete analytical treatment. There exists another, "operational," line of research, initiated in Donoho [11]. The spirit of the operational approach is perfectly well illustrated by the main result of the latter paper stating that when recovering the linear form of unknown signal x known to belong to a given convex compact set $\mathcal{X}$ via indirect Gaussian observation $\omega = Ax + \xi$,

$\xi \sim \mathcal{N}(0, I)$, the worst-case, over $x \in \mathcal{X}$, risk of an affine in ω estimate yielded by optimal solution to an explicit convex optimization problem is within the Factor 1.2 of the minimax optimal risk. Subsequent "operational" literature is of similar spirit: both the recommended estimate and its risk are given by an efficient computation (typically, stem from solutions to explicit convex optimization problems); in addition, in good situations we know in advance that the resulting risk, whether large or small, is nearly minimax optimal. The explanation power of operational results is almost nonexisting; as a compensation, the scope of operational results is usually much wider than the one of analytical results. For example, the just cited result of D. Donoho imposes no restrictions on A and $\mathcal{X}$, except for convexity and compactness of $\mathcal{X}$; in contrast, all known to us analytical results on the same problem subject $(A, \mathcal{X})$ to severe structural restrictions.

In terms of the outlined "descriptive – operational" dichotomy, our paper is operational. For instance, in the problem of estimating linear functional of signal x affinely parameterising the parameters θ, Θ of sub-Gaussian distribution we started with, we allow for quite general affine mapping $x \to (\theta, \Theta)$ and for general enough signal set $\mathcal{X}$, the only restrictions on $\mathcal{X}$ being convexity and compactness. This generality allows to handle problems too difficult for "closed analytical form" design and analysis, and even problems which, from the traditional viewpoint, may seem meaningless. To illustrate the latter point, let the signal underlying sub-Gaussian observation is just the pair of "sub-Gaussianity parameters:" $x = (\theta, \Theta)$, and let $G(x)$ be a linear function of the Θ-component of x. At the first glance, the resulting estimation problem is senseless: a sub-Gaussian, with parameters (θ, Θ), distribution P does "remember" θ, but *does not* "remember" Θ, so that even complete knowledge of the distribution of our observation, not speaking about knowledge of just a sample drawn from P, does not allow to recover Θ exactly. With the descriptive approach with its primary focus on rates of convergence, this observation would be enough to qualify the problem as meaningless – what can be said about rate of convergence when there cannot be convergence at all? By contrast, there is no reason to reject the problem as meaningless within operational approach: we can still apply the machinery we develop below to build a "presumably good" estimate of the functional of interest. This estimate can provide us with perhaps incomplete, but still meaningful information on the functional of interest. Indeed, depending on $\mathcal{X}$, some nontrivial information on the Θ-component of $x = (\theta, \Theta) \in \mathcal{X}$ may be "stored" in θ, and observations do provide us with a nontrivial information on θ. The bottom line is: with the operational approach, there is no need to decide in advance which estimation problems are, and which are not meaningful: we can apply our estimation machinery to the problem at hand to get both the estimate and an upper bound on its ϵ-risk.

Technically, the approach we use in this paper combines the machinery developed in Goldenshluger, Juditsky and Nemirovski [20,28] and the Cramer-type techniques for upper-bounding the risk of an affine estimate developed in Juditsky and Nemirovski [27].[1] On the other hand, this approach can also be viewed as "computation-friendly" extension of theoretical results on "Cramer tests" supplied by Birgé [2–5] in conjunction with techniques of Donoho, Liu and MacGibbon [14], Donoho and Nussbaum [15], Donoho and Liu [12,13], Donoho [11], Butucea and Meziani [8], which exploits the most attractive, in our opinion, feature of this line of research – potential applicability to a wide variety of observation schemes and (convex) signal sets $\mathcal{X}$.

[1] To handle quadratic in observation estimates we treat them as affine functions of "quadratic lifting" $\omega^+ = [\omega; 1][\omega; 1]^T$ of the actual observation ω.

The rest of the paper is organized as follows. In Section 2 we, following Juditsky and Nemirovski [28], describe the families of distributions we are working with. In the nutshell, these are families of distributions specified by a given bound $\Phi(f;\mu)$ on the logarithmic moment-generating function:

$$\forall (x\in\mathcal{X}, P\in\mathcal{P}_x): \ln\big(\mathbf{E}_{\omega\sim P}\big\{e^{f^T\omega}\big\}\big)\leq \Phi\big(f;\mu(x)\big)\quad \forall (f\in\mathcal{F}),$$

where continuous *convex-concave* function $\Phi(f;\mu):\mathcal{F}\times\mathcal{M}\to\mathbf{R}$, closed convex symmetric w.r.t. the origin set $\mathcal{F}$, closed convex set $\mathcal{M}$, and affine mapping $x\mapsto\mu(x):\mathcal{X}\to\mathcal{M}$ are given "parameters." The simplest example is presented by the family of sub-Gaussian distributions with sub-Gaussianity parameters affinely parameterized by signals, where $\mathcal{F}=\mathbf{R}^m$, $\mathcal{M}$ is comprised of all pairs $\mu=(\theta,\Theta)$ with $\theta\in\mathbf{R}^m$ and positive semidefinite symmetric $m\times m$ matrices Θ, and $\Phi(f;\mu)=\Phi(f;\theta,\Theta)=f^T\theta+\frac{1}{2}f^T\Theta f$. We build our estimate and study its general properties in Section 3. Then in Section 4 we discuss applications to estimating linear forms of parameters of sub-Gaussian distributions. In Section 5 we apply the proposed construction to estimating quadratic forms of parameters of Gaussian and discrete distributions. When estimating quadratic functionals, upper risk bounds for the developed estimators are not supported by strong "generic" optimality results available in the case of linear functional estimation. Nevertheless, in some important situations which allow for analytical study (cf., e.g., Donoho and Nussbaum [15], Klemelä [31]) the proposed estimates are nearly minimax optimal. Moreover, near-optimality properties of these estimates can be studied numerically. To illustrate the performance of the proposed approach we describe results of some preliminary numerical experiments in which we compare the bounds on the risk of estimates supplied by our machinery with (numerically computed) lower bounds on the minimax risk. Proofs are relegated to the supplement paper Juditsky and Nemirovski [30].

Notation. In what follows, $\mathbf{R}^n$ and $\mathbf{S}^n$ stand for the spaces of real n-dimensional vectors and real symmetric $n\times n$ matrices, respectively; both spaces are equipped with the standard inner products, x^Ty, resp., $\mathrm{Tr}(XY)$. Relation $A\succeq B$ ($A\succ B$) means that A, B are symmetric matrices of the same size such that $A-B$ is positive semidefinite (resp., positive definite). We denote $\mathbf{S}^n_+=\{S\in\mathbf{S}^n: S\succeq 0\}$ and $\mathbf{S}^n_{++}=\mathrm{int}\,\mathbf{S}^n_+=\{S\in\mathbf{S}^n: S\succ 0\}$.

We use "MATLAB notation:" $[X_1;\dots;X_k]$ means vertical concatenation of matrices $X_1,\dots,X_k$ of the same width, and $[X_1,\dots,X_k]$ means horizontal concatenation of matrices $X_1,\dots,X_k$ of the same height. In particular, for reals $x_1,\dots,x_k$, $[x_1;\dots;x_k]$ is a k-dimensional column vector with entries $x_1,\dots,x_k$.

For probability distributions $P_1,\dots,P_K$, $P_1\times\cdots\times P_K$ is the product distribution on the direct product of the corresponding probability spaces; when $P_1=\cdots=P_K$, we denote $P_1\times\cdots\times P_K$ by P^K or $[P]^K$.

Given positive integer d, $\theta\in\mathbf{R}^d$, $\Theta\in\mathbf{S}^d_+$, we denote by $\mathcal{SG}(\theta,\Theta)$ the family of all sub-Gaussian, with parameters (θ,Θ), probability distributions, that is, the family of all Borel probability distributions P on $\mathbf{R}^d$ such that

$$\forall f\in\mathbf{R}^d: \ln\big(\mathbf{E}_{\omega\sim P}\{e^{f^T\omega}\big)\leq f^T\theta+\frac{1}{2}f^T\Theta f.$$

We use shorthand notation $\omega\sim\mathcal{SG}(\theta,\Theta)$ to express the fact that the probability distribution of random vector ω belongs to the family $\mathcal{SG}(\theta,\Theta)$.

2. Simple families of probability distributions

Let

- $\mathcal{F}$, $0 \in \operatorname{int}\mathcal{F}$, be a closed convex set in $\Omega = \mathbf{R}^m$ symmetric w.r.t. the origin,
- $\mathcal{M}$ be a closed convex set in some $\mathbf{R}^n$,
- $\Phi(f;\mu) : \mathcal{F} \times \mathcal{M} \to \mathbf{R}$ be a continuous function convex in $f \in \mathcal{F}$ and concave in $\mu \in \mathcal{M}$.

Following Juditsky and Nemirovski [28], we refer to $\mathcal{F}$, $\mathcal{M}$, $\Phi(\cdot,\cdot)$ satisfying the above restrictions as to *regular data*. Regular data $\mathcal{F}$, $\mathcal{M}$, $\Phi(\cdot,\cdot)$ define the family $\mathcal{S} = \mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ of Borel probability distributions P on Ω such that

$$\exists \mu \in \mathcal{M} : \forall f \in \mathcal{F} : \quad \ln\left(\int_\Omega \exp\left\{f^T\omega\right\} P(d\omega)\right) \le \Phi(f;\mu). \tag{2.1}$$

We say that distributions satisfying (2.1) are *simple*. Given regular data $\mathcal{F}$, $\mathcal{M}$, $\Phi(\cdot,\cdot)$, we refer to $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ as to *simple* family of distributions associated with the data $\mathcal{F}$, $\mathcal{M}$, Φ. Standard examples of simple families are supplied by "good observation schemes," as defined in Juditsky and Nemirovski [27], Goldenshluger, Juditsky and Nemirovski [20], and include the families of Gaussian, Poisson and discrete distributions. For other instructive examples and an algorithmic "calculus" of simple families, the reader is referred to Juditsky and Nemirovski [28]. We present here three examples of simple families which we use in the sequel.

2.1. Sub-Gaussian, Poisson, and discrete distributions

1. When $\mathcal{F} = \Omega = \mathbf{R}^d$, $\mathcal{M}$ is a closed convex subset of $\mathcal{G}_d = \{\mu = (\theta, \Theta) : \theta \in \mathbf{R}^d, \Theta \in \mathbf{S}^d_+\}$, and $\Phi(f;\theta,\Theta) = \theta^T f + \frac{1}{2} f^T \Theta f$, $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ is comprised of all sub-Gaussian distributions P on $\mathbf{R}^d$ with sub-Gaussianity parameters from $\mathcal{M}$. In particular, $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ contains all normal distributions $\mathcal{N}(\theta, \Theta)$ with $(\theta, \Theta) \in \mathcal{M}$.
2. When $\mathcal{F} = \mathbf{R}^d$, $\Omega = \mathbf{Z}^d_+$ (nonnegative integer vectors in $\mathbf{R}^d$), $\mathcal{M} = \mathbf{R}^d_+$ and $\Phi(f;\mu) = \sum_{i=1}^d \mu_i[\mathrm{e}^{f_i} - 1]$, $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ contains distributions of d-dimensional random vectors $\omega = [\omega_1; \dots; \omega_d]$ with independent across i entries $\omega_i \sim \mathrm{Poisson}(\mu_i)$.
3. When $\mathcal{F} = \mathbf{R}^d$, $\Omega = \{e_1, \dots, e_d\} \subset \mathbf{R}^d$, where e_i are basic orths,[2] $\mathcal{M} = \{\mu \in \mathbf{R}^d : \mu \ge 0, \sum_i \mu_i = 1\}$, and $\Phi(f;\mu) = \ln(\sum_{i=1}^d \mu_i \mathrm{e}^{f_i})$, $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ contains all discrete probability distributions on d-element set Ω.

2.2. Quadratically lifted Gaussian observations

Let $\mathcal{V}$ be a nonempty convex compact subset of $\mathbf{S}^d_+$. This set gives rise to the family $\mathcal{P}[\mathcal{V}]$ of distributions of *quadratic liftings* $[\zeta;1][\zeta;1]^T$ of random vectors $\zeta \sim \mathcal{N}(\theta, \Theta)$ with $\theta \in \mathbf{R}^d$ and

[2]The just defined Ω as a convenient for us "encoding" of the set of realizations of a discrete random variable taking d possible values.

$\Theta \in \mathcal{V}$. Let us build regular data such that the associated simple family of distributions contains $\mathcal{P}[\mathcal{V}]$. To this end, we select $\Theta_* \in \mathbf{S}^d_{++}$ and $\delta \geq 0$ such that for all $\Theta \in \mathcal{V}$ one has

$$\Theta \preceq \Theta_* \quad \text{and} \quad \|\Theta^{1/2}\Theta_*^{-1/2} - I\| \leq \delta, \tag{2.2}$$

where $\|\cdot\|$ is the spectral norm; under these restrictions, the smaller are Θ_* and δ, the better. Observe that for all $\Theta \in \mathcal{V}$, we have $0 \preceq \Theta_*^{-1/2}\Theta\Theta_*^{-1/2} \preceq I$. Hence,

$$\|\Theta^{1/2}\Theta_*^{-1/2}\|^2 = \|\Theta_*^{-1/2}\Theta^{1/2}\|^2 = \|\Theta_*^{-1/2}\Theta^{1/2}[\Theta_*^{-1/2}\Theta^{1/2}]^T\| = \|\Theta_*^{-1/2}\Theta\Theta_*^{-1/2}\| \leq 1,$$

and we lose nothing when assuming from now on that $\delta \in [0, 2]$. The required regular data are given by the following proposition.

Proposition 2.1. *In the just described situation, let* $\gamma \in (0, 1)$,

$$\mathcal{Z}^+ = \{Z \in \mathbf{S}^{d+1} : Z_{d+1,d+1} = 1\}, \qquad \mathcal{H}_\gamma = \{H \in \mathbf{S}^d : -\gamma\Theta_*^{-1} \preceq H \preceq \gamma\Theta_*^{-1}\}$$

and let $\mathcal{F} = \mathbf{R}^d \times \mathcal{H}_\gamma$, $\mathcal{M}^+ = \mathcal{V} \times \mathcal{Z}^+$. *We set*

$$\begin{aligned}
\Phi(h, H; \Theta, Z) &= \Upsilon(H, \Theta) + \Gamma(h, H, Z),\\
\Upsilon(H, \Theta) &= -\frac{1}{2}\ln\mathrm{Det}\big(I - \Theta_*^{1/2}H\Theta_*^{1/2}\big) + \frac{1}{2}\mathrm{Tr}\big([\Theta - \Theta_*]H\big)\\
&\quad + \frac{\delta(2+\delta)}{2(1 - \|\Theta_*^{1/2}H\Theta_*^{1/2}\|)}\|\Theta_*^{1/2}H\Theta_*^{1/2}\|_F^2,\\
\Gamma(h, H; Z) &= \frac{1}{2}\mathrm{Tr}\left(Z\left[\left[\begin{array}{c|c} H & h \\ \hline h^T & \end{array}\right] + [H, h]^T\big[\Theta_*^{-1} - H\big]^{-1}[H, h]\right]\right).
\end{aligned} \tag{2.3}$$

Then

(i) $\mathcal{F}, \mathcal{M}^+, \Phi$ *form a regular data, and for every* $(\theta, \Theta) \in \mathbf{R}^d \times \mathcal{V}$ *it holds for all* $(h, H) \in \mathcal{F}$:

$$\ln\big(\mathbf{E}_{\zeta\sim\mathcal{N}(\theta,\Theta)}\{e^{h^T\zeta + \frac{1}{2}\zeta^T H\zeta}\}\big) \leq \Phi\big(h, H; \Theta, [\theta; 1][\theta; 1]^T\big). \tag{2.4}$$

(ii) *Besides this, function* $\Phi(h, H; \Theta, Z)$ *is coercive in the convex argument: whenever* $(\Theta, Z) \in \mathcal{M}^+$, $(h_i, H_i) \in \mathcal{F}$ *and* $\|(h_i, H_i)\| \to \infty$ *as* $i \to \infty$, *we have* $\Phi(h_i, H_i; \Theta, Z) \to \infty$.

For proof, see Section B.1 of the supplement paper.

2.3. Quadratically lifted discrete observations

Consider a random variable $\zeta \in \mathbf{R}^d$ taking values e_i, $i = 1, \dots, d$, where e_i are standard basic orths in $\mathbf{R}^d$ (as was already mentioned, this is a convenient way to encode random variable taking d possible values). Same as in 2.1.3, we identify the probability distribution P_μ of such variable with a point $\mu = [\mu_1; \dots; \mu_d]$ from the d-dimensional probabilistic simplex $\Delta^d = \{\nu \in \mathbf{R}^d_+ : \sum_{i=1}^d \nu_i = 1\}$ where $\mu_i = \mathrm{Prob}\{\zeta = e_i\}$. Let now $\zeta^K = (\zeta_1, \dots, \zeta_K)$ with ζ_k drawn independently across k from P_μ, and let

$$\omega[\zeta^K] = \frac{2}{K(K-1)} \sum_{1 \le j < j \le K} \omega_{ij}[\zeta^K], \quad \omega_{ij}[\zeta^K] = \frac{1}{2}[\zeta_i \zeta_j^T + \zeta_j \zeta_i^T], 1 \le i < j \le K. \quad (2.5)$$

We are about to point our regular data such that the associated simple family of distributions contains the distributions of the "quadratic lifts" $\omega[\zeta^K]$ of random vectors ζ^K.

Proposition 2.2. *Let $\mathcal{F} = \mathbf{S}^d$,*

$$\mathbf{\Delta}^d = \left\{ Z \in \mathbf{S}^d : Z_{ij} \ge 0 \ \forall i, j, \sum_{i,j} Z_{ij} = 1 \right\}. \quad (2.6)$$

and let $\mathcal{Z}^d$ be a set of all positive semidefinite matrices from $\mathbf{\Delta}^d$. Denote

$$\Phi(H; Z) = \ln\left(\sum_{i,j=1}^m Z_{ij} \exp\{H_{ij}\} \right) : \mathbf{S}^d \times \mathbf{\Delta}^d \to \mathbf{R}, \quad (2.7)$$

so that $\Phi(\cdot;\cdot)$ is convex-concave on $\mathbf{S}^d \times \mathbf{\Delta}^d$. We set

$$\Phi_M(H; Z) = M\Phi(H/M; Z), \quad M \in \mathbf{Z}_+.$$

Then for $M = M(K) = \lfloor K/2 \rfloor$,

$$\ln\left(\mathbf{E}_{\zeta^K \sim P_\mu^K}\left\{\exp\left\{\mathrm{Tr}\left(H\omega\left[\zeta^K\right]\right)\right\}\right\}\right) \le \Phi_M\left(H; \mu\mu^T\right). \quad (2.8)$$

In other words, the simple family $\mathcal{S}[\mathcal{F}, \mathcal{Z}^d, \Phi_{\lfloor K/2 \rfloor}]$ contains distributions of all random variables $\omega[\zeta^K]$ with $\zeta \sim P_\mu$, $\mu \in \Delta^d$.

For proof, see Section B.2 of the supplement paper.

3. Estimating linear forms

3.1. Situation and goal

Consider the situation as follows: given are Euclidean spaces $\mathcal{E}_F, \mathcal{E}_M, \mathcal{E}_X$ along with

- regular data $\mathcal{F} \subset \mathcal{E}_F, \mathcal{M} \subset \mathcal{E}_M, \Phi(\cdot;\cdot) : \mathcal{F} \times \mathcal{M} \to \mathbf{R}$,
- a nonempty convex compact set $\mathcal{X} \subset \mathcal{E}_X$,
- an affine mapping $x \mapsto \mathcal{A}(x) : \mathcal{E}_X \to \mathcal{E}_M$ such that $\mathcal{A}(\mathcal{X}) \subset \mathcal{M}$,

- a vector $g \in \mathcal{E}_X$ and a constant c specifying the linear form $G(x) = \langle g, x\rangle + c : \mathcal{E}_X \to \mathbf{R}$,[3]
- a tolerance $\epsilon \in (0, 1)$ and a positive integer number K of available observations.

Let $\mathcal{P}$ be the family of all Borel probability distributions on $\mathcal{E}_F$. Given a random observation $\omega^K = (\omega_1, \dots, \omega_K)$ with i.i.d. components

$$\omega_k \sim P(\cdot), \quad k \leq K, \tag{3.1}$$

where $P \in \mathcal{P}$ is *associated* with unknown signal x known to belong to $\mathcal{X}$, we want to recover $G(x)$. Here "association" of a probability distribution P with a signal $x \in \mathcal{X}$ means that

$$P \in \mathcal{P}_x := \left\{P : \ln\left(\int_{\mathcal{E}_F} \mathrm{e}^{\langle f,\omega\rangle} P(d\omega)\right) \leq \Phi\big(f; \mathcal{A}(x)\big)\ \forall f \in \mathcal{F}\right\} \tag{3.2}$$

Note that the problem we have just posed is a special case of the general estimation problem described in the Introduction, the case where the functional to be recovered is affine, and the families $\mathcal{P}_x$ of probability distributions associated with signals $x \in \mathcal{X}$ are defined by (3.2).

3.2. The construction

Let us set

$$\mathcal{F}_K^+ = \big\{\big(f^K, \alpha\big) : f^K = (f_1, \dots, f_K) \in \mathcal{E}_F^K := \mathcal{E}_F \times \cdots \times \mathcal{E}_F, \alpha > 0, f_k/\alpha \in \mathcal{F}, 1 \leq k \leq K\big\}$$

so that $\mathcal{F}_K^+$ is a nonempty convex set in $\mathcal{E}_F^K \times \mathbf{R}_+$, and let

$$\Psi_{+,K}\big(f^K, \alpha\big) = \max_{x \in \mathcal{X}}\left[\alpha \sum_{k=1}^K \Phi\big(f_k/\alpha, \mathcal{A}(x)\big) - G(x)\right] : \mathcal{F}_K^+ \to \mathbf{R},$$

$$\Psi_{-,K}\big(f^K, \alpha\big) = \max_{x \in \mathcal{X}}\left[\alpha \sum_{k=1}^K \Phi\big(-f_k/\alpha, \mathcal{A}(x)\big) + G(x)\right] : \mathcal{F}_K^+ \to \mathbf{R},$$

so that $\Psi_{\pm,K}$ are convex real-valued functions on $\mathcal{F}_K^+$ (recall that Φ is convex-concave and continuous on $\mathcal{F} \times \mathcal{M}$, while $\mathcal{A}(\mathcal{X})$ is a compact subset of $\mathcal{M}$). These functions give rise to convex functions $\widehat{\Psi}_\pm : \mathcal{E}_F^K \to \mathbf{R}$ given by

$$\widehat{\Psi}_{+,K}\big(f^K\big) := \inf_\alpha\big\{\Psi_{+,K}\big(f^K, \alpha\big) + \alpha \ln(2/\epsilon) : \big(f^K, \alpha\big) \in \mathcal{F}_K^+\big\},$$

$$\widehat{\Psi}_{-,K}\big(f^K\big) := \inf_\alpha\big\{\Psi_{-,K}\big(f^K, \alpha\big) + \alpha \ln(2/\epsilon) : \big(f^K, \alpha\big) \in \mathcal{F}_K^+\big\}$$

[3]from now on, $\langle u, v\rangle$ denotes the inner product of vectors u, v belonging to a Euclidean space; what is this space, it always will be clear from the context.

and to convex optimization problem

$$\mathrm{Opt} = \min_{f^K} \left\{ \widehat{\Psi}_K(f^K) := \frac{1}{2}\big[\widehat{\Psi}_{+,K}(f^K) + \widehat{\Psi}_{-,K}(f^K)\big] \right\}, \tag{3.3}$$

With our approach, a "presumably good" estimate of $G(x)$ and its risk are given by an optimal (or nearly so) solution to the latter problem. The corresponding result is as follows.

Proposition 3.1. *In the situation of Section 3.1, let Φ satisfy the relation*

$$\Phi(0;\mu) \geq 0 \quad \forall \mu \in \mathcal{M}. \tag{3.4}$$

Then

$$\begin{aligned} \widehat{\Psi}_{+,K}(f^K) &:= \inf_{\alpha} \big\{ \Psi_{+,K}(f^K, \alpha) + \alpha \ln(2/\epsilon) : (f^K, \alpha) \in \mathcal{F}_K^+ \big\} \\ &= \max_{x \in \mathcal{X}} \inf_{\alpha : (f^K, \alpha) \in \mathcal{F}_K^+} \left[\alpha \sum_{k=1}^K \Phi\big(f_k/\alpha, \mathcal{A}(x)\big) - G(x) + \alpha \ln(2/\epsilon) \right], \end{aligned} \tag{3.5}$$

$$\begin{aligned} \widehat{\Psi}_{-,K}(f^K) &:= \inf_{\alpha} \big\{ \Psi_{-,K}(f^K, \alpha) + \alpha \ln(2/\epsilon) : (f^K, \alpha) \in \mathcal{F}_K^+ \big\} \\ &= \max_{x \in \mathcal{X}} \inf_{\alpha : (f^K, \alpha) \in \mathcal{F}_K^+} \left[\alpha \sum_{k=1}^K \Phi\big(-f_k/\alpha, \mathcal{A}(x)\big) + G(x) + \alpha \ln(2/\epsilon) \right], \end{aligned} \tag{3.6}$$

and the functions $\widehat{\Psi}_{\pm,K}(\cdot)$ are convex real-valued. Furthermore, a feasible solution $\bar{f}^K$, $\bar{\varkappa}$, $\bar{\rho}$ to the system of convex constraints

$$\widehat{\Psi}_{+,K}(f^K) \leq \rho - \varkappa, \qquad \widehat{\Psi}_{-,K}(f^K) \leq \rho + \varkappa \tag{3.7}$$

in variables f^K, ρ, $\varkappa$ induces K-observation estimate

$$\widehat{G}(\omega) = \sum_{k=1}^K \langle \bar{f}_k, \omega_k \rangle + \bar{\varkappa}, \tag{3.8}$$

of $G(x)$, $x \in \mathcal{X}$, with ϵ-risk at most $\bar{\rho}$:

$$\mathrm{Risk}_\epsilon\big(\widehat{G}(\cdot)|\mathcal{X}\big) \leq \bar{\rho}, \tag{3.9}$$

where ϵ-risk Risk_ϵ *is defined by* (1.1), *and the families $\mathcal{P}_x$, $x \in \mathcal{X}$, are given by* (3.2). *Relation* (3.7) (*and thus – the risk bound* (3.9)) *clearly holds true when $\bar{f}^K$ is a candidate solution to problem* (3.3) *and*

$$\bar{\rho} = \widehat{\Psi}_K(\bar{f}^K), \qquad \bar{\varkappa} = \frac{1}{2}\big[\widehat{\Psi}_{-,K}(\bar{f}^K) - \widehat{\Psi}_{+,K}(\bar{f}^K)\big].$$

As a result, by properly selecting $\bar{f}^K$ we can make (*an upper bound on*) *the ϵ-risk of estimate* (3.8) *arbitrarily close to* Opt, *and equal to* Opt *when optimization problem* (3.3) *is solvable.*

For proof, see Section B.3 of the supplement paper.

Let us make the following simple and useful observation: the functions $\Psi_{\pm,K}(f^K,\alpha)$ are convex and symmetric w.r.t. permutations of components $f_1,\dots,f_K$ in $f^K=(f_1,\dots,f_K)$; as a result, the functions $\widehat{\Psi}_{\pm,K}(f^K)$ also are convex and symmetric w.r.t. permutations of $f_1,\dots,f_K$. Consequently, whenever a collection $(\bar f^K,\bar\varkappa,\bar\rho)$ is feasible for the system of constraints (3.7), so is the collection $(\widetilde{f}^K,\bar\varkappa,\bar\rho)$, where $\widetilde{f}^K$ is a permutation of $\bar f^K$; since the constraints in question are convex, it follows that replacing the components $\bar f_1,\dots,\bar f_K$ by their mean, that is, passing from $(\bar f^K,\bar\varkappa,\bar\rho)$ to the collection $(\widehat{f}^K,\bar\varkappa,\bar\rho)$ with $\widehat{f}_k=\frac{1}{K}\sum_{k=1}^K\bar f_k$, $k=1,\dots,K$, we get a collection satisfying (3.7). The bottom line is that we lose nothing when restricting ourselves to collections f^K with identical components. Denoting by f/K the common value of these components, Proposition 3.1 becomes the statements as follows.

Proposition 3.2. *In the situation described in Section 3.1, let Φ satisfy the relation (3.4). Setting*

$$\begin{aligned}\mathcal{F}^+&=\big\{(f,\alpha):\alpha>0,\,f/\alpha\in\mathcal{F}\big\},\\ \Psi_+(f,\alpha)&=\max_{x\in\mathcal{X}}\big[\alpha\Phi\big(f/\alpha,\mathcal{A}(x)\big)-G(x)\big]:\mathcal{F}^+\to\mathbf{R},\\ \Psi_-(f,\alpha)&=\max_{x\in\mathcal{X}}\big[\alpha\Phi\big(-f/\alpha;\mathcal{A}(x)\big)+G(x)\big]:\mathcal{F}^+\to\mathbf{R},\end{aligned}$$

the functions $\widehat{\Psi}_\pm:\mathcal{E}_F\to\mathbf{R}$,

$$\begin{aligned}\widehat{\Psi}_+(f)&:=\inf_\alpha\big\{\Psi_+(f,\alpha)+K^{-1}\alpha\ln(2/\epsilon):(f,\alpha)\in\mathcal{F}^+\big\}\\ &=\max_{x\in\mathcal{X}}\inf_{\alpha:(f,\alpha)\in\mathcal{F}^+}\big[\alpha\Phi\big(f/\alpha,\mathcal{A}(x)\big)-G(x)+K^{-1}\alpha\ln(2/\epsilon)\big],\\ \widehat{\Psi}_-(f)&:=\inf_\alpha\big\{\Psi_-(f,\alpha)+K^{-1}\alpha\ln(2/\epsilon):(f,\alpha)\in\mathcal{F}^+\big\}\\ &=\max_{x\in\mathcal{X}}\inf_{\alpha:(f,\alpha)\in\mathcal{F}^+}\big[\alpha\Phi\big(-f/\alpha,\mathcal{A}(x)\big)+G(x)+K^{-1}\alpha\ln(2/\epsilon)\big]\end{aligned}$$

are convex and real valued. Furthermore, let $\bar f$, $\bar\varkappa$, $\bar\rho$ be a feasible solution to the system of convex constraints

$$\widehat{\Psi}_+(f)\le\rho-\varkappa,\qquad\widehat{\Psi}_-(f)\le\rho+\varkappa\tag{3.10}$$

in variables f, ρ, $\varkappa$. Then, setting

$$\widehat{G}\big(\omega^K\big)=\Big\langle\bar f,\frac{1}{K}\sum_{k=1}^K\omega_k\Big\rangle+\bar\varkappa,\tag{3.11}$$

we get an estimate of $G(x)$, $x\in\mathcal{X}$, via K-repeated observation $\omega^K=(\omega_1,\dots,\omega_K)$ with independent across k components $\omega_k\sim P$ with ϵ-risk at most $\bar\rho$, meaning that whenever a Borel probability distribution P is associated with $x\in\mathcal{X}$ in the sense of (3.2), one has

$$\operatorname{Prob}_{\omega^K\sim P^K}\big\{\omega^K:\big|\widehat{G}\big(\omega^K\big)-G(x)\big|>\bar\rho\big\}\le\epsilon.$$

Relation (3.10) *clearly holds true when* $\bar{f}$ *is a candidate solution to the convex optimization problem*

$$\mathrm{Opt} = \min_f \left\{ \widehat{\Psi}(f) := \frac{1}{2}\big[\widehat{\Psi}_+(f) + \widehat{\Psi}_-(f)\big] \right\} \tag{3.12}$$

and

$$\bar{\rho} = \widehat{\Psi}(\bar{f}), \qquad \bar{\varkappa} = \frac{1}{2}\big[\widehat{\Psi}_-(\bar{f}) - \widehat{\Psi}_+(\bar{f})\big].$$

As a result, properly selecting $\bar{f}$, *we can make* (*an upper bound on*) *the* ϵ*-risk of estimate* $\widehat{G}(\cdot)$ *arbitrarily close to* Opt, *and equal to* Opt *when optimization problem* (3.12) *is solvable. Finally, the optimal value in* (3.12) *is exactly the same as the optimal value in* (3.3).

4. Application: Estimating linear form of parameters of sub-Gaussian distributions

For numerical illustration of the subsequent results, see Section A of the supplement paper.

4.1. Situation and result

We are about to apply construction form Section 3 in the situation where our observation is sub-Gaussian with parameters affinely parameterized by signal x, and our goal is to recover a linear function of x. Specifically, consider the situation described in Section 3, with the data as follows:

- $\mathcal{F} = \mathcal{E}_F = \mathbf{R}^d$, $\mathcal{M} = \mathcal{E}_M = \mathbf{R}^d \times \mathbf{S}^d_+$, $\Phi(f; \theta, \Theta) = f^T\theta + \frac{1}{2} f^T \Theta f : \mathbf{R}^d \times (\mathbf{R}^d \times \mathbf{S}^d_+) \to \mathbf{R}$ (so that $\mathcal{S}[\mathcal{F}, \mathcal{M}, \Phi]$ is the family of all sub-Gaussian distributions on $\mathbf{R}^d$);
- $\mathcal{X} \subset \mathcal{E}_X = \mathbf{R}^{n_x}$ is a nonempty convex compact set, and
- $\mathcal{A}(x) = (Ax + a, M(x))$, where A is $d \times n_x$ matrix, and $M(x)$ is affinely depending on x symmetric $d \times d$ matrix such that $M(x)$ is $\succeq 0$ when $x \in \mathcal{X}$,
- $G(x)$ is an affine function on $\mathcal{E}_X$.

Same as in Section 3, our goal is to recover the value of a given linear function $G(y) = g^T y + c$ at unknown signal $x \in \mathcal{X}$ via K-repeated observation $\omega^K = (\omega_1, \dots, \omega_K)$ with ω_k drawn, independently across k, from a distribution P which is associated with x, which now means "is sub-Gaussian with parameters $(Ax + a, M(x))$." We refer to *Gaussian case* as to the special case of the just described problem, where the distribution P associated with signal x is exactly $\mathcal{N}(Ax + a, M(x))$.

In the case in question $\Phi(0; \theta, \Theta) = 0$, so that (3.4) takes place, and the left-hand sides in the constraints (3.10) are

$$\begin{aligned}\widehat{\Psi}_+(f) &= \max_{x\in\mathcal{X}} \inf_{\alpha>0} \left\{ f^T[Ax + a] + \frac{1}{2\alpha} f^T M(x) f + K^{-1}\alpha \ln(2/\epsilon) - G(x) \right\} \\ &= \max_{x\in\mathcal{X}} \left\{ \big[2K^{-1}\ln(2/\epsilon) f^T M(x) f\big]^{1/2} + f^T Ax - G(x) \right\} + a^T f, \end{aligned} \tag{4.1}$$

$$\begin{aligned}\widehat{\Psi}_-(f) &= \max_{x\in\mathcal{X}}\inf_{\alpha>0}\left\{-f^T[Ax+a]+\frac{1}{2\alpha}f^TM(x)f+K^{-1}\alpha\ln(2/\epsilon)+G(x)\right\}\\ &= \max_{x\in\mathcal{X}}\left\{\left[2K^{-1}\ln(2/\epsilon)f^TM(x)f\right]^{1/2}-f^TAx+G(x)\right\}-a^Tf. \qquad (4.2)\end{aligned}$$

We arrive at the following version of Proposition 3.2.

Proposition 4.1. *In the situation described above, given $\epsilon\in(0,1)$, let $\bar{f}$ be a feasible solution to the convex optimization problem*

$$\mathrm{Opt}(K)=\min_{f\in\mathbf{R}^d}\left\{\widehat{\Psi}(f):=\frac{1}{2}\left[\widehat{\Psi}_+(f)+\widehat{\Psi}_-(f)\right]\right\}, \qquad (4.3)$$

where $\widehat{\Psi}_\pm(\cdot)$ are given by (4.1), (4.2). Setting

$$\bar{\varkappa}=\frac{1}{2}\left[\widehat{\Psi}_-(\bar{f})-\widehat{\Psi}_+(\bar{f})\right],\qquad \bar{\rho}=\widehat{\Psi}(\bar{f}),$$

the ϵ-risk of the affine estimate

$$\widehat{G}(\omega^K)=\frac{1}{K}\sum_{k=1}^{K}\bar{f}^T\omega_k+\bar{\varkappa},$$

taken w.r.t. the data listed in the beginning of this section, is at most $\bar{\rho}$.

It is immediately seen that optimization problem (4.3) is solvable, provided that $\bigcap_{x\in\mathcal{X}}\mathrm{Ker}(M(x))=\{0\}$, and an optimal solution f_* to the problem, taken along with

$$\varkappa_*=\frac{1}{2}\left[\widehat{\Psi}_-(f_*)-\widehat{\Psi}_+(f_*)\right], \qquad (4.4)$$

yields the affine estimate

$$\widehat{G}_*(\omega)=\frac{1}{K}\sum_{i=1}^{K}f_*^T\omega_i+\varkappa_*$$

with ϵ-risk, w.r.t. the data listed in the beginning of this section, at most $\mathrm{Opt}(K)$.

Consistency. We can easily answer the natural question "when the proposed estimation scheme is consistent", meaning that for every $\epsilon\in(0,1)$, it allows to achieve arbitrarily small ϵ-risk, provided that K is large enough. Specifically, if we denote $G(x)=g^Tx+c$, from Proposition 4.1 it is immediately seen that a sufficient condition for consistency is the existence of $\bar{f}\in\mathbf{R}^d$ such that $\bar{f}^TAx=g^Tx$ for all $x\in\mathcal{X}-\mathcal{X}$, or, equivalently, that g is orthogonal to the intersection of the kernel of A with the linear span of $\mathcal{X}-\mathcal{X}$. Indeed, under this assumption, for every fixed $\epsilon\in(0,1)$ we clearly have $\lim_{K\to\infty}\widehat{\Phi}(\bar{f})=0$, implying that $\lim_{K\to\infty}\mathrm{Opt}(K)=0$, with $\widehat{\Psi}$ and $\mathrm{Opt}(K)$ given by (4.1), (4.2), (4.3). The condition in question is necessary for consistency as well, since when the condition is violated, we have $Ax' = Ax''$ for properly selected $x', x'' \in \mathcal{X}$ with $G(x') \neq G(x'')$, making low risk recovery of $G(x)$, $x \in \mathcal{X}$, impossible already in the case of zero noise, where an observation stemming from signal $x \in \mathcal{X}$ is identically equal to $Ax + a$.[4]

4.2. Direct product case

Further simplifications are possible in the *direct product case*, where, in addition to what was assumed in the beginning of Section 4,

- $\mathcal{E}_X = \mathcal{E}_U \times \mathcal{E}_V$ and $\mathcal{X} = U \times V$, with convex compact sets $U \subset \mathcal{E}_U = \mathbf{R}^{n_u}$ and $V \subset E_V = \mathbf{R}^{n_v}$,
- $\mathcal{A}(x = (u, v)) = [Au + a, M(v)] : U \times V \to \mathbf{R}^d \times \mathbf{S}^d$, with $M(v) \succeq 0$ for $v \in V$,
- $G(x = (u, v)) = g^T u + c$ depends solely on u.

It is immediately seen that in the direct product case problem (4.3) reads

$$\begin{aligned} \mathrm{Opt} = \min_{f \in \mathbf{R}^d} \bigg\{ & \frac{1}{2}\big[\phi_U\big(A^T f - g\big) + \phi_U\big(-A^T f + g\big)\big] \\ & + \max_{v \in V} \big[2K^{-1} \ln(2/\epsilon) f^T M(v) f\big]^{1/2} \bigg\}, \end{aligned} \tag{4.5}$$

where

$$\phi_U(h) = \max_{u \in U} u^T h.$$

Assuming $\bigcap_{v \in V} \mathrm{Ker}(M(v)) = \{0\}$, the problem is solvable, and its optimal solution f_* gives rise to the affine estimate

$$\widehat{G}_*(\omega^K) = \frac{1}{K} \sum_{k=1}^{K} f_*^T \omega_k + \varkappa_*, \quad \varkappa_* = \frac{1}{2}\big[\phi_U\big(-A^T f_* + g\big) - \phi_U\big(A^T f_* - g\big)\big] - a^T f_* + c,$$

with ϵ-risk $\leq$ Opt.

Near-optimality. In addition to the assumption that we are in the direct product case, assume for the sake of simplicity, that $M(v) \succ 0$ whenever $v \in V$. In this case, (4.3) reads

$$\begin{aligned} \mathrm{Opt} = \min_f \max_{v \in V} \bigg\{ & S(f, v) := \frac{1}{2}\big[\phi_U\big(A^T f - g\big) \\ & + \phi_U\big(-A^T f + g\big)\big] + \big[2K^{-1} \ln(2/\epsilon) f^T M(v) f\big]^{1/2} \bigg\}, \end{aligned}$$

[4] Note that in the Gaussian case with $M(x)$ depending on x the above condition is, in general, not necessary for consistency, since a nontrivial information on x (and thus on $G(x)$) can, in principle, be extracted from the covariance matrix $M(x)$ which can be estimated from observations.

whence, taking into account that $S(f, v)$ clearly is convex in f and concave in v, while V is a convex compact set, by Sion–Kakutani theorem we get also

$$\mathrm{Opt} = \max_{v \in V} \left\{ \mathrm{Opt}(v) = \min_f \left[\frac{1}{2} \left[\phi_U\left(A^T f - g\right) + \phi_U\left(-A^T f + g\right) \right] + \left[2K^{-1} \ln(2/\epsilon) f^T M(v) f \right]^{1/2} \right] \right\}. \tag{4.6}$$

Now consider the problem of recovering $g^T u$ from observation ω_k, $1 \le k \le K$, independently of each other sampled from $\mathcal{N}(Au + a, M(v))$, where unknown u is known to belong to U and $v \in V$ is known. Let $\rho_\epsilon(v)$ be the minimax ϵ-risk of the recovery:

$$\rho_\epsilon(v) = \inf_{\widehat{G}(\cdot)} \left\{ \rho : \mathrm{Prob}_{\omega^K \sim [\mathcal{N}(Au+a, M(v))]^K} \left\{ \omega^K : \left| \widehat{G}\left(\omega^K\right) - g^T u \right| > \rho \right\} \le \epsilon \ \forall u \in U \right\},$$

where inf is taken over all Borel functions $\widehat{G}(\cdot) : \mathbf{R}^{Kd} \to \mathbf{R}$. Invoking Juditsky and Nemirovski [27], Proposition 4.1, it is immediately seen that whenever $\epsilon < \frac{1}{2}$, one has

$$\rho_\epsilon(v) \ge \frac{q_{\mathcal{N}}(1-\epsilon)}{\sqrt{2\ln(2/\epsilon)}} \mathrm{Opt}(v),$$

where $q_{\mathcal{N}}(s)$ is the s-quantile of the standard normal distribution. Since the family of all sub-Gaussian, with parameters $(Au + a, M(v))$, $u \in U$, $v \in V$, distributions on $\mathbf{R}^d$ contains all Gaussian distributions $\mathcal{N}(Au + a, M(v))$ induced by $(u, v) \in U \times V$, we arrive at the following conclusion.

Proposition 4.2. *In the just described situation, the minimax optimal ϵ-risk*

$$\mathrm{Risk}_\epsilon^{\mathrm{opt}}(K) = \inf_{\widehat{G}(\cdot)} \mathrm{Risk}_\epsilon\left(\widehat{G}(\cdot)\right),$$

of recovering $g^T u$ from K-repeated i.i.d. sub-Gaussian, with parameters $(Au + a, M(v))$, $(u, v) \in U \times V$, random observations is within a moderate factor of the upper bound Opt *on the ϵ-risk, taken w.r.t. the same data, of the affine estimate $\widehat{G}_*(\cdot)$ yielded by an optimal solution to* (4.5). *Namely,*

$$\mathrm{Opt} \le \frac{\sqrt{2\ln(2/\epsilon)}}{q_{\mathcal{N}}(1-\epsilon)} \mathrm{Risk}_\epsilon^{\mathrm{opt}}$$

with the "near-optimality factor" $\frac{\sqrt{2\ln(2/\epsilon)}}{q_{\mathcal{N}}(1-\epsilon)} \to 1$ *as* $\epsilon \to 0$.[5]

[5] It is worth mentioning that in a more general setting of "good observation schemes," described in Juditsky and Nemirovski [27], the ϵ-risk Opt of the affine estimate constructed following the rules in Section 3 satisfies the bound $\mathrm{Opt} \le \frac{2\ln(2/\epsilon)}{\ln(\frac{1}{4\epsilon})} \mathrm{Risk}_\epsilon^{\mathrm{opt}}$, where $\mathrm{Risk}_\epsilon^{\mathrm{opt}}$ is the corresponding minimax ϵ-risk. In particular, this is what happens when the constructions from Section 3 are applied to the families of Poisson or Discrete distributions, see Section 2.1, rather than to the family of sub-Gaussian distributions.

5. Quadratic lifting and estimating quadratic forms

In this section, we apply the approach in Section 3 to the situation where, given an i.i.d. sample $\zeta^K = [\zeta_1; \dots; \zeta_K]$, $\zeta_i \in \mathbf{R}^d$, with distribution P_x of ζ_k depending on an unknown "signal" $x \in \mathcal{X}$, our goal is to estimate a quadratic functional $q(x) = x^T Qx + c^T x$ of the signal. We consider two situations – the *Gaussian case*, where P_x is a Gaussian distribution with parameters affinely depending on x, and *discrete case* where $\mathcal{X}$ is a probabilistic simplex, and P_x is a discrete distribution corresponding to the probabilistic vector Ax, A being a given stochastic matrix. Our estimation strategy is to apply the techniques developed in Section 3 to *quadratic liftings* ω of actual observations ζ (e.g., $\omega_k = (\zeta_k, \zeta_k\zeta_k^T)$ in the Gaussian case), so that the resulting estimates are affine functions of ω's. We first focus on implementing this program in the Gaussian case.

5.1. Estimating quadratic forms, Gaussian case

In this section, we focus on the problem as follows. Given are

- a nonempty bounded set $U \subset \mathbf{R}^m$ and a nonempty convex compact set $V \subset \mathbf{R}^k$,
- an affine mapping $v \mapsto M(v) : \mathbf{R}^k \to \mathbf{S}^d$ which maps V onto convex compact subset $\mathcal{V}$ of $\mathbf{S}^d_+$;
- an affine mapping $u \mapsto A[u; 1] : \mathbf{R}^m \to \Omega = \mathbf{R}^d$, where A is a given $d \times (m+1)$ matrix,
- a "functional of interest"

$$F(u, v) = [u; 1]^T Q[u; 1] + q^T v : \mathbf{R}^m \times \mathbf{R}^k \to \mathbf{R}, \tag{5.1}$$

  where Q and q are known $(m+1) \times (m+1)$ symmetric matrix and k-dimensional vector, respectively.
- a tolerance $\epsilon \in (0, 1)$.

We observe an i.i.d. sample $\zeta^K = [\zeta_1; \dots; \zeta_K]$, $\zeta_i \in \mathbf{R}^d$, with Gaussian distribution $P_{u,v}$ of ζ_i depending on an unknown "signal" (u, v) known to belong to $U \times V$: $P_{u,v} = \mathcal{N}(A[u; 1], M(v))$. Our goal is to estimate $F(u, v)$ from observation ζ^K.

The ϵ-risk $\mathrm{Risk}_\epsilon(\widehat{G})$ of a candidate estimate $\widehat{G}(\cdot)$ – a Borel real-valued function on $\mathbf{R}^{Kd}$ – is defined as the smallest ρ such that

$$\forall \big((u, v) \in U \times V\big) : \mathrm{Prob}_{\zeta^K \sim P^K_{u,v}} \big\{ \big|\widehat{G}\big(\zeta^K\big) - F(u, v)\big| > \rho \big\} \le \epsilon.$$

5.1.1. *Construction*

Our course of actions is as follows.

- We specify convex compact subset $\mathcal{Z} \subset \mathbf{S}^{m+1}$ such that

$$\forall u \in U : [u; 1][u; 1]^T \in \mathcal{Z} \subset \mathcal{Z}^+ = \big\{ Z \in \mathbf{S}^{m+1}_+ : Z_{m+1,m+1} = 1 \big\}, \tag{5.2}$$

  matrix $\Theta_* \in \mathbf{S}^d$ and real $\delta \in [0, 2]$ such that $\Theta_* \succ 0$ and

$$\forall \Theta \in \mathcal{V} : \Theta \preceq \Theta_* \quad \text{and} \quad \big\| \Theta^{1/2}\Theta_*^{-1/2} - I \big\| \le \delta; \tag{5.3}$$

  (cf. Section 2.2).

- We set $x(u,v)=(v,[u;1][u;1]^T)$, and

$$X=\{(v,[u;1][u;1]^T):u\in U,v\in V\},$$

so that

$$X\subset\mathcal{X}:=V\times\mathcal{Z}\subset\mathcal{E}_X:=\mathbf{R}^k\times\mathbf{S}^{m+1}.$$

We select $\gamma\in(0,1)$ and set

$$\begin{array}{ll}\mathcal{H}_\gamma=\{H\in\mathbf{S}^d:-\gamma\Theta_*^{-1}\preceq H\preceq\gamma\Theta_*^{-1}\}, & \mathcal{F}=\mathbf{R}^d\times\mathcal{H}_\gamma\subset\mathcal{E}_F=\mathbf{R}^d\times\mathbf{S}^d,\\ \mathcal{M}=\mathcal{V}\times B\mathcal{Z}^+B^T\subset\mathcal{E}_M=\mathbf{S}^d\times\mathbf{S}^{d+1}, & B=[A;e_{m+1}^T],\end{array}\tag{5.4}$$

where e_{m+1} is the $(m+1)$th basis orth in $\mathbf{R}^{m+1}$.
- When adding to the above entities function $\Phi(\cdot;\cdot)$, as defined in (2.3), we conclude by Proposition 2.1 that $\mathcal{M}$, $\mathcal{F}$ and $\Phi(\cdot;\cdot)$ form a regular data such that for all $(u,v)\in U\times V$ and $(h,H)\in\mathcal{F}$,

$$\ln\bigl(\mathbf{E}_{\zeta\sim P_{u,v}}\{\exp\{\langle(h,H),(\zeta,\zeta\zeta^T)\rangle\}\}\bigr)\le\Phi\bigl(h,H;M(v),B[u;1][u;1]^TB^T\bigr),\tag{5.5}$$

where the inner product $\langle\cdot,\cdot\rangle$ on $\mathcal{E}_F$ is defined as $\langle(h,H),(g,G)\rangle=h^Tg+\frac{1}{2}\mathrm{Tr}(HG)$, so that $\langle(h,H),(\zeta,\zeta\zeta^T)\rangle=h^T\zeta+\frac{1}{2}\zeta^TH\zeta$.

Observe that $\mathcal{A}(x=(v,\underbrace{[u;1][u;1]^T}_{Z}))=(M(v),BZB^T)$ is an affine mapping which maps $\mathcal{X}$ into $\mathcal{M}$, and $G(x):\mathcal{E}_X\to\mathbf{R}$,

$$G(x)=\mathrm{Tr}(QZ)+q^Tv=[u;1]^TQ[u;1]+q^Tv$$

is a linear functional on $\mathcal{E}_X$.

As a result of the above steps, we get at our disposal entities $\mathcal{E}_X$, $\mathcal{E}_M$, $\mathcal{E}_F$, $\mathcal{F}$, $\mathcal{M}$, Φ, $\mathcal{X}$, $\mathcal{A}(\cdot)$, $G(\cdot)$ and ϵ participating in the setup described in Section 3.1, and it is immediately seen that these entities meet all the requirements imposed by this setup. The bottom line is that the estimation problem stated in the beginning of this section reduces to the problem considered in Section 3.

5.1.2. *The result*

When applying to the resulting data Proposition 3.2 (which is legitimate, since Φ in (2.3) clearly satisfies (3.4)), we arrive at the result as follows:

Proposition 5.1. *In the just described situation, let us set*

$$
\begin{aligned}
\widehat{\Psi}_+(h,H) = \max_{(v,Z)\in V\times\mathcal{Z}} \inf_{\substack{\alpha>0,\\ -\gamma\alpha\Theta_*^{-1}\preceq H\preceq\gamma\alpha\Theta_*^{-1}}} &\left\{\alpha\Phi\left(\frac{h}{\alpha},\frac{H}{\alpha};M(v),BZB^T\right)\right.\\
&\left. - G(v,Z)+\frac{\alpha}{K}\ln\left(\frac{2}{\epsilon}\right)\right\},\\
\widehat{\Psi}_-(h,H) = \max_{(v,Z)\in V\times\mathcal{Z}} \inf_{\substack{\alpha>0,\\ -\gamma\alpha\Theta_*^{-1}\preceq H\preceq\gamma\alpha\Theta_*^{-1}}} &\left\{\alpha\Phi\left(-\frac{h}{\alpha},-\frac{H}{\alpha};M(v),BZB^T\right)\right.\\
&\left. + G(v,Z)+\frac{\alpha}{K}\ln\left(\frac{2}{\epsilon}\right)\right\}.
\end{aligned}
\tag{5.6}
$$

so that the functions $\widehat{\Psi}_\pm(h,H):\mathbf{R}^d\times\mathbf{S}^d\to\mathbf{R}$ *are convex. Whenever* $\bar{h},\bar{H},\bar{\rho},\bar{\varkappa}$ *form a feasible solution to the system of convex constraints*

$$
\widehat{\Psi}_+(h,H)\le\rho-\varkappa,\ \widehat{\Psi}_-(h,H)\le\rho+\varkappa \tag{5.7}
$$

in variables $(h,H)\in\mathbf{R}^d\times\mathbf{S}^d$, $\rho\in\mathbf{R}$, $\varkappa\in\mathbf{R}$, *setting*

$$
\widehat{G}\big(\zeta^K:=(\zeta_1,\dots,\zeta_K)\big)=\frac{1}{K}\sum_{i=1}^K\left[h^T\zeta_i+\frac{1}{2}\zeta_i^TH\zeta_i\right]+\bar{\varkappa}, \tag{5.8}
$$

we get an estimate of the functional of interest $F(u,v)=[u;1]^TQ[u;1]+q^Tv$ *via* K *independent observations*

$$
\zeta_i\sim\mathcal{N}\big(A[u;1],M(v)\big),\quad i=1,\dots,K,
$$

with ϵ*-risk not exceeding* $\bar{\rho}$:

$$
\forall(u,v)\in U\times V:\mathrm{Prob}_{\zeta^K\sim[\mathcal{N}(A[u;1],M(v))]^K}\left\{\left|F(u,v)-\widehat{G}\big(\zeta^K\big)\right|>\bar{\rho}\right\}\le\epsilon. \tag{5.9}
$$

In particular, setting for $(h,H)\in\mathbf{R}^d\times\mathbf{S}^d$

$$
\bar{\rho}=\frac{1}{2}\big[\widehat{\Psi}_+(h,H)+\widehat{\Psi}_-(h,H)\big],\qquad \bar{\varkappa}=\frac{1}{2}\big[\widehat{\Psi}_-(h,H)-\widehat{\Psi}_+(h,H)\big], \tag{5.10}
$$

we obtain an estimate (5.8) *with* ϵ*-risk not exceeding* $\bar{\rho}$.

For proof, see Section B.4 of the supplement paper.

Remark 5.1. In the situation described in the beginning of this section, let a set $W\subset U\times V$ be given, and assume we are interested in recovering functional of interest (5.1) at points $(u,v)\in$

W only. When reducing the "domain of interest" to W, we hopefully can reduce the ϵ-risk of recovery. Assuming that we can point out a convex compact set $\mathcal{W} \subset V \times \mathcal{Z}$ such that

$$(u, v) \in W \quad \Rightarrow \quad \big(v, [u; 1][u; 1]^T\big) \in \mathcal{W},$$

it can be straightforwardly verified that in this case the conclusion of Proposition 5.1 remains valid when the set $V \times \mathcal{Z}$ in (5.6) is replaced with $\mathcal{W}$, and the set $U \times V$ in (5.9) is replaced with W. This modification enlarges the feasible set of (5.7) and thus reduces the attainable risk bound.

5.1.3. *Illustrating example*: *Energy estimation from direct observations*

To illustrate Proposition 5.1, consider the simple situation as follows: Given observation

$$\zeta = u + \xi, \quad \xi \sim \mathcal{N}(0, \Theta I_m) \tag{5.11}$$

with u known to belong to the spherical layer $U = \{u \in \mathbf{R}^m : r^2 \le u^T u \le R^2\}$ and Θ known to be diagonal with diagonal entries in the segment $[\theta\sigma^2, \sigma^2]$, we want to recover $F(u) = u^T u$. Here r, R, θ, σ are known, with $0 \le r < R$, $\theta \in [0, 1]$, and $\sigma > 0$. The situation is covered by the setup of Section 5.1, where we set $V = \{v \in \mathbf{R}^m : \theta \le v_i \le 1, i \le m\}$, $M(v) = \sigma^2 \operatorname{Diag}\{v\}$,[6] $A[u; 1] = u$, and $K = 1$.

In the situation just described, Proposition 5.1 boils down to the following.

A. We lose nothing when restricting ourselves with estimates of the form

$$\widehat{G}(\zeta) = \frac{\eta}{2}\zeta^T\zeta + \varkappa, \tag{5.12}$$

with properly selected scalars η and $\varkappa$. Specifically, η and $\varkappa$ are supplied by the convex optimization problem (with just 3 variables α, β, η)

$$\mathrm{Opt} = \min_{\alpha,\beta,\eta}\left\{\widehat{\Psi}(\alpha, \beta, \eta) = \frac{1}{2}\big[\widehat{\Psi}_+(\alpha, \eta) + \widehat{\Psi}_-(\beta, \eta)\big] : \sigma^2|\eta| < \min[\alpha, \beta]\right\}, \tag{5.13}$$

where

$$\begin{aligned}
\widehat{\Psi}_+(\alpha, \eta) &= -\frac{m\alpha}{2}\ln\big(1 - \sigma^2\eta/\alpha\big) + \frac{m}{2}\sigma^2(1-\theta)\max[-\eta, 0] + \frac{m\delta(2+\delta)\sigma^4\eta^2}{2(\alpha - \sigma^2|\eta|)} \\
&\quad + \max_{r^2 \le t \le R^2}\left[\left[\frac{\alpha\eta}{2(\alpha - \sigma^2\eta)} - 1\right]t\right] + \alpha\ln(2/\epsilon), \\
\widehat{\Psi}_-(\beta, \eta) &= -\frac{m\beta}{2}\ln\big(1 + \sigma^2\eta/\beta\big) + \frac{m}{2}\sigma^2(1-\theta)\max[\eta, 0] + \frac{m\delta(2+\delta)\sigma^4\eta^2}{2(\beta - \sigma^2|\eta|)} \\
&\quad + \max_{r^2 \le t \le R^2}\left[\left[-\frac{\beta\eta}{2(\beta + \sigma^2\eta)} + 1\right]t\right] + \beta\ln(2/\epsilon),
\end{aligned} \tag{5.14}$$

[6]Here and in what follows $\operatorname{Diag}\{A_1, A_2, \dots, A_k\}$ stands for a block-diagonal matrix with diagonal blocks $A_1, A_2, \dots, A_k$.

with $\delta = 1 - \sqrt{\theta}$. Specifically, the η-component of a feasible solution to (5.13) augmented by the quantity

$$\varkappa = \frac{1}{2}\big[\widehat{\Psi}_-(\beta,\eta) - \widehat{\Psi}_+(\alpha,\eta)\big]$$

yields estimate (5.12) with ϵ-risk on U not exceeding $\widehat{\Psi}(\alpha,\beta,\eta)$; note that this risk can be made arbitrarily close to Opt.

B. In the simple situation in question, it is easy to extract from (5.13) analytical bounds on ϵ-risk of our estimate.[7] To simplify our life, we restrict ourselves with two extreme cases: the one where the (diagonal) covariance matrix of noise is known exactly ($\theta = 1$) and the one when all we know is that this matrix is diagonal $\preceq \sigma^2 I_m$ ($\theta = 0$). Assume in addition that $r = 0$.

B.1: $\theta = 1, r = 0$. In this case, one has

$$\mathrm{Opt} \le 2\sigma\sqrt{m\sigma^2 + 2R^2}\sqrt{\ln(2/\epsilon)}. \tag{5.15}$$

B.2: $\theta = 0, r = 0$. One has

$$\mathrm{Opt} \le 2\sigma\sqrt{m\sigma^2 + 2R^2}\sqrt{\ln(2/\epsilon)} + 3\sigma^2 m. \tag{5.16}$$

The simple "energy estimation" problem we consider in this section is well studied – in this setting the interplay between the dimension m of signal, the range of noise intensity σ^2 and parameters R, r, ϵ can be studied analytically to provide provably optimal, up to absolute constant factors, estimates. Note that bounds (5.15) and (5.16) for the "extreme cases" are nearly minimax optimal up to logarithmic in $1/\epsilon$ factor when R is not "too small" – $R^2 \ge O(1)\sigma^2\sqrt{m}$ when $\theta = 1$, and $R^2 \ge O(1)\sigma^2 m$ when $\theta = 0$ – otherwise the trivial estimate $\widehat{G}(\zeta) \equiv 0$ is minimax optimal. They attest that risk bounds (5.12) yielded by the optimal solution to (5.13) have similar near-optimality characteristics in this case. A nice property of the proposed approach is that (5.13) automatically takes care of the parameters and results in estimates with near-optimal performance, as is witnessed by the numerical results we present in Section C of the supplement paper.

5.1.4. *Discussion*

Repeated observations. When estimating quadratic forms from K-repeated observations $\zeta^K = [\zeta_1; \dots; \zeta_K]$ with i.i.d. ζ_i we applied "literally" the construction of Section 3, thus restricting ourselves with estimates affine in quadratic liftings $\omega_i = (\zeta_i, \zeta_i\zeta_i^T)$ of ζ_i's. As an alternative to such "basic" approach, let us consider estimates which are affine in the "full" quadratic lifting $\omega = (\zeta^K, \zeta^K[\zeta^K]^T)$ of ζ^K, thus extending the family of candidate estimates (what is affine in $\omega_1, \dots, \omega_K$, is affine in ω, but not vice versa, unless $K = 1$). Note that this alternative is covered by our approach – all we need, is to replace the original components d, $M(\cdot)$, $\mathcal{V}$, A of the setup

[7]For detailed justification of what follows, see Section C of the supplement paper.

of this section with their extensions

$$d^+ = Kd, \qquad M^+(v) = \mathrm{Diag}\{\underbrace{M(v), \ldots, M(v)}_{K}\},$$

$$\mathcal{V}^+ = M^+(V) = \{\Theta = \mathrm{Diag}\{M(v), \ldots, M(v)\}, v \in V\}, \qquad A^+ = [A; \ldots; A],$$

and set K to 1.

It is easily seen that such modification can only reduce the risk of the resulting estimates, the price being the increase in design dimension (and thus in computational complexity) of the optimization problems yielding the estimates. To illustrate the difference between two approaches, consider the problem of energy estimation from observation (5.11) discussed in the previous section where Θ is (unknown) diagonal matrix with diagonal entries from the range $[0, \sigma^2]$, and a priori information about u is that $\|u\|_2 \le R$ for some known R. Assume that $m \ge 16 \ln(2/\epsilon)$, where $\epsilon \in (0, 1)$ is a given reliability tolerance and that $R^2 \ge m\sigma^2$. Under these assumptions one can easily verify that in the single-observation case the ϵ-risks of both the "plug-in" estimate $\zeta^T\zeta$ and of the estimate yielded by the proposed approach are, up to absolute constant factors, the same as the minimax optimal ϵ-risk, namely, $O(1)\mathcal{R}$, $\mathcal{R} = \sigma^2 m + \sigma R\sqrt{\ln(2/\epsilon)}$ (cf. (5.16)). Now let us look at the case $K = 2$ where we observe two independent copies, ζ_1 and ζ_2, of observation (5.11). Here, the ϵ-risks of the "naive" plug-in estimate $\frac{1}{2}[\zeta_1^T\zeta_1 + \zeta_2^T\zeta_2]$, and of the estimate obtained by applying our "basic" approach with $K = 2$ are just by absolute constant factors better than in the single-observation case – both these risks still are $O(1)\mathcal{R}$. In contrast to this, an "intelligent" plug-in 2-observation estimate $\zeta_1^T\zeta_2$ has risk $O(1)\sigma(R + \sigma\sqrt{m})\sqrt{\ln(2/\epsilon)}$ whenever $R \ge 0$, which is much smaller than $\mathcal{R}$ when $m \gg \ln(2/\sigma)$ and $R\sqrt{\ln(2/\epsilon)} \ll \sigma m$. It is easily seen that with the outlined alternative implementation, our approach also results in estimate with "correct" ϵ-risk $O(1)\sigma(R + \sigma\sqrt{m})\sqrt{\ln(2/\epsilon)}$. It should be mentioned that the phenomenon in question stems from uncertainty in Θ.

Adaptation. When analysing performance of estimation routines in the minimax framework we are only interested in the worst-case performance (risk) over signals from a given (possibly large) signal set. Were we told in advance that the actual signal belongs to a much smaller set, we typically could recover the functional of interest with essentially smaller risk. Intrinsic conservatism and lack of flexibility, often considered as principal shortcomings of the minimax approach, become even more obvious when estimating quadratic functionals. For example, in the energy recovery problem from Section 5.1.3 with $U = \{u : u^T u \le R^2\}$, the focus of nearly minimax optimal estimates built in Section 5.1.3 is on recovering energy of order of R^2. When restricting ourselves, for the sake of simplicity, to the case of $\mathcal{N}(0, \sigma^2 I_m)$ noise with known σ (i.e., with $\theta = 1$), the worst case ϵ-risk of our estimate is $\approx [\sigma^2\sqrt{m} + \sigma R]$, where $\approx$ stands for "up to logarithmic in $1/\epsilon$ factors." At the same time, the ϵ-risk of the simplest under the circumstances estimate $\zeta^T\zeta - \sigma^2 m$ at signal u is $\approx [\sigma^2 m + \sigma\|u\|_2]$, so that the second estimate is basically as good in the worst case as the first one, but is much better suited for estimating energy of "weak signals" with energy $\ll R^2$.

We are about to explain that in the problem we are interested in this "built-in" shortcoming of the minimax approach can be (at least, to some extent) cured by passing from the original to the straightforward adaptive version of our procedures.[8] Specifically, in the situation described in the beginning of Section 5.1, assume that for some integer L we have at our disposal "filtration" $[\varnothing \neq]U_1 \subset U_2 \subset \cdots \subset U_L \equiv U$ and $[\varnothing \neq]V_1 \subset V_2 \subset \cdots \subset V_L \equiv V$ which are lifted to filtration $\mathcal{Z}_1 \subset \cdots \subset \mathcal{Z}_L \equiv \mathcal{Z}$ and $\mathcal{V}_1 \subset \cdots \subset \mathcal{V}_L \equiv \mathcal{V}$ required by construction from Section 5.1.1. In other words, $\mathcal{Z}_\ell$ are convex compact subsets of $\mathcal{Z}^+$ such that $[u;1][u;1]^T \in \mathcal{Z}_\ell$ whenever $u \in U_\ell$, and $\mathcal{V}_\ell$ are convex compact subsets of $\mathbf{S}^d_+$ such that $M(v) \in \mathcal{V}_\ell$ whenever $v \in V_\ell$. Besides this, we equip sets $\mathcal{V}_\ell$ with positive definite matrices $\Theta_{*,\ell}$ and reals $\delta_\ell \in [0,2]$ such that $\Theta_{*,1} \preceq \Theta_{*,2} \preceq \ldots \preceq \Theta_L$, $\delta_1 \leq \delta_2 \leq \cdots \leq \delta_L$, and relation (5.3) holds true with $V_\ell, \Theta_{*,\ell}$ and δ_ℓ in the role of $\mathcal{V}, \Theta_*, \delta$. Applying the machinery from Section 5.1.1 to $U_\ell, \ldots, \delta_\ell$ in the role of $U, \ldots, \delta$, and $\epsilon_+ = \epsilon/L$ in the role of ϵ, we get estimates $\widehat{G}_\ell(\zeta^K)$ and risk bounds $\bar{\rho}_\ell$, $\ell \leq L$, such that

$$\begin{aligned} &\forall (u,v) \in U_\ell \times V_\ell, \\ &\qquad \mathrm{Prob}_{\zeta^K \sim [\mathcal{N}(A[u;1],M(v))]^K}\left\{\left|F(u,v) - \widehat{G}_\ell\left(\zeta^K\right)\right| > \bar{\rho}_\ell\right\} \leq \epsilon/L, \quad 1 \leq \ell \leq L. \end{aligned}$$

Assuming w.l.o.g. that $\bar{\rho}_1 \leq \bar{\rho}_2 \leq \cdots \leq \bar{\rho}_L$, let us assemble the estimates $\widehat{G}_\ell$ as follows. Given observation ζ^K, we compute $g_\ell := \widehat{G}_\ell(\zeta^K)$ and call index ℓ ζ^K*-good*, if the segments $\Delta_r(\zeta^K) = [\widehat{G}_r(\zeta^K) - \bar{\rho}_r, \widehat{G}_r(\zeta^K) + \bar{\rho}_r]$, $\ell \leq r \leq L$, have a point in common. Good indexes do exist (e.g., $\ell = L$); we select the smallest of them, let it be denoted by $\underline{\ell} = \underline{\ell}(\zeta^K)$, and take the midpoint $\widehat{G}_*(\zeta^K)$ of the (nonempty!) segment $\bigcap_{\underline{\ell} \leq r \leq L} \Delta_r(\zeta^K)$, as the adaptive estimate of $F(u,v)$. By standard arguments (cf. Lepskii [39]), the resulting estimate satisfies the relation

$$\forall (\ell \leq L, u, v \in U_\ell \times V_\ell) : \mathrm{Prob}_{\zeta^K \sim [\mathcal{N}(A[u;1],M(v))]^K}\left\{\left|F(u,v) - \widehat{G}_*\left(\zeta^K\right)\right| > \bar{\rho}_\ell\right\} \leq \epsilon, \quad (5.17)$$

whence

$$\begin{aligned} \mathrm{Risk}_\epsilon[\widehat{G}_* | U_\ell \times v_\ell] := \min\Big\{\rho : &\mathrm{Prob}_{\zeta^K \sim [\mathcal{N}(A[u;1],M(v))]^K}\left\{\left|F(u,v) - \widehat{G}_*\left(\zeta^K\right)\right| > \bar{\rho}_\ell\right\} \leq \epsilon \\ &\forall (u,v) \in U_\ell \times V_\ell\Big\} \\ \leq{}& 2\bar{\rho}_\ell, \quad 1 \leq \ell \leq L. \end{aligned}$$

That is, the ϵ-risk of the aggregated estimate on *each signal set* $X_\ell = U_\ell \times V_\ell$ is within factor 2 of the ϵ/L-risk of the estimate provided by our procedure as applied to the set X_ℓ.

Indeed, let us fix $\ell \in \{1,\ldots,L\}$, and let the signal underlying our observation be $(u,v) \in U_\ell \times V_\ell$, so that the distribution $P_{u,v}$ of the observation stemming from (u,v) is the distribution of K independent across $k \leq K$ blocks $\zeta_k \sim \mathcal{N}(A[u;1], M(v))$. For $\ell \leq r \leq L$, let $\mathcal{E}_r$ be the event $\{\zeta^K : |\widehat{G}_r(\zeta^K) - F(u,v)| \leq \bar{\rho}_r\}$. Since $(u,v) \in U_r \times V_r$ for $r \geq \ell$, the $P_{u,v}$-probability of $\mathcal{E}_r$ is at least $1 - \epsilon/L$, implying that the probability of the event $\mathcal{E} = \bigcap_{r \geq \ell} \mathcal{E}_\ell$ is at least $1 - \epsilon$. Assume that $\zeta^K \in \mathcal{E}$. Then the segments $\Delta_r(\zeta^K)$, $\ell \leq r \leq L$, have a point in common,

[8] The adaptive estimate described below is in fact an adopted for our purposes simplified version of adaptive estimation routines from Klemelä [31], Butucea and Meziani [8]. Of course, one can also consider other approaches to improving estimate performance beyond the minimax setting, e.g., those utilizing "pilot" plug-in estimate as in Laurent and Massart [35] or implementing estimation in relative risk scales (cf. Juditsky and Nemirovski [29]) just to mention a few. However, these developments are beyond the scope of this paper.

namely, $F(u,v)$, and ℓ is ζ^K-good. Consequently, $\underline{\ell}(\zeta^K)\le\ell$, meaning that $\widehat{G}_*(\zeta^K)\in\Delta_\ell(\zeta^K)$ by construction of $\widehat{G}_*$. Since we are in the case when the latter segment contains $F(u,v)$, we get $|F(u,v)-\widehat{G}_*(\zeta^K)|\le 2\bar{\rho}_\ell$, as claimed in (5.17).

Note that the "cost" of the above adaptation amounts to the necessity to tune estimates $\widehat{G}_\ell$ to reliability tolerance ϵ/L rather than ϵ; as is immediately seen from (5.6), to get this improvement in reliability, it suffices to increase the number of observations by factor $\ln(2L/\epsilon)/\ln(2/\epsilon)$. And of course similar construction can be applied to all estimation problems considered in this paper, not only to problem posed in Section 5.1.

Coming back to the example from Section 5.1.3 and assuming for the sake of simplicity that $r=0$, the simplest way to implement adaptive estimation is to use the filtration $U_\ell=2^{\ell-L}R$, $V_\ell=V=\{v\in\mathbf{R}^m:\theta\le v_i\le 1\}$, select L resulting in "small" R_1, specifically, $R_1\le\sigma\sqrt{m}$, and set $\mathcal{Z}_\ell=\{Z\in\mathbf{S}^{m+1}_+:Z_{m+1,m+1}=1,\mathrm{Tr}(Z)\le R_\ell^2+1\}$. Utilizing (5.15) and (5.16), we conclude that with this filtration we obtain estimate $\widehat{F}(\cdot)$ of $F(u)=u^Tu$ which ensures signal-dependent risk bound

$$\begin{aligned}
&\forall\big(u\in\mathbf{R}^m,\|u\|\le R, v\in V\big):\\
&\mathrm{Risk}_\epsilon(u,v):=\min\big\{\rho:\mathrm{Prob}_{\zeta^K\sim[\mathcal{N}(A[u;1],M(v))]^K}\big\{\big|F(u,v)-\widehat{G}_*\big(\zeta^K\big)\big|>\rho\big\}\le\epsilon\big\}\\
&\qquad\qquad\le\begin{cases}2\sigma\sqrt{m\sigma^2+2u^Tu}\sqrt{\ln(2L/\epsilon)}, & \text{in the case of } \mathit{B.1},\\ 8\sigma\sqrt{m\sigma^2+2u^Tu}\sqrt{\ln(2L/\epsilon)}+3\sigma^2m, & \text{in the case of } \mathit{B.2},\end{cases}\\
&L=\rfloor\log_2(1+R/\sigma)\lfloor.
\end{aligned}$$

In the case of *B.1*, the resulting risk bound *for every u with $\|u\|\le R$* is basically the same as for the standard estimate $\zeta^T\zeta-\sigma^2m$. This being said. note that the latter estimate, in contrast to the first one, is an "ad hoc" construction with the scope restricted to the case of direct observations $\zeta=u+\xi$, $\xi\sim\mathcal{N}(0,\sigma^2I_m)$, with known σ.

5.1.5. *Consistency*

Note that risk bounds of Proposition 5.1 are not supported by generic optimality as it was the case in the problem of linear functional estimation in Section 3. One of the reasons for this is that "quadratic estimates" built in Section 5.1.1 are suboptimal for certain types of geometry of the signal set U even in the problem of signal energy estimation from direct observations (see, e.g., Cai and Low [9,10]). Nevertheless, in some important cases the constructed estimates are nearly minimax optimal. For instance, consider the problem of estimating a quadratic function $F(u)=\sum_{i=1}^m q_iu_i^2$, $q_i\ge 0$, from observation $\zeta=u+\xi$, $\xi\sim\mathcal{N}(0,\sigma^2I_m)$, in the setting described in Donoho and Nussbaum [15] where the signal set U is *quadratically convex*, meaning that $u=\{u\in\mathbf{R}^m:[u_1^2;\dots;u_m^2]\in\mathcal{T}\}$, where the set $\mathcal{T}\subset\mathbf{R}^m_+$ is convex, compact, and *monotone* (i.e., $0\le t'\le t$, $t\in\mathcal{T}$). The performance of an estimator is measured by the maximal over U expected recovery error

$$\mathrm{Risk}\big(\widehat{F}(\cdot)|U\big)=\sup_{u\in U}\mathbf{E}_{\zeta\sim\mathcal{N}(u,\sigma^2I)}\big\{\big(\widehat{F}(\omega)-F(u)\big)^2\big\}.$$

It can be shown that in this case the risk bounds yielded by Proposition 5.1 are within logarithmic in $1/\epsilon$ factor (stemming from passing from Risk to Risk_ϵ) of the minimax risk (cf. Theorem 6 of Donoho and Nussbaum [15]).

Now we are about to present a simple sufficient condition for the estimator suggested by Proposition 5.1 to be consistent, in the sense of Section 4. Specifically, assume that

A.1. $V = \{\bar{v}\}$ is a singleton such that $M(\bar{v}) \succ 0$, which allows to satisfy (2.2) with $\Theta_* = M(\bar{v})$ and $\delta = 0$, same as allows to assume w.l.o.g. that

$$F(u, v) = [u; 1]^T Q[u; 1], \qquad G\big(x = (v, Z)\big) = \mathrm{Tr}(QZ);$$

A.2. The first m columns of the $d \times (m+1)$ matrix A are linearly independent.

By A.2, the columns of $(d+1) \times (m+1)$ matrix B, see (5.4), are linearly independent, so that we can find $(m+1) \times (d+1)$ matrix C such that $CB = I_{m+1}$. Let us define $(\bar{h}, \bar{H}) \in \mathbf{R}^d \times \mathbf{S}^d$ from the relation

$$\left[\begin{array}{c|c} \bar{H} & \bar{h} \\ \hline \bar{h}^T & \end{array}\right] = 2\big[C^T QC\big]^o, \tag{5.18}$$

where for $(d+1) \times (d+1)$ matrix S, S^o is the matrix obtained from S by replacing the entry $S_{d+1,d+1}$ with zero. The consistency of our estimation procedure is given by the following simple statement.

Proposition 5.2. *In the just described situation and under assumptions* A.1–A.2, *given* $\epsilon \in (0, 1)$, *consider the estimate*

$$\widehat{G}_K\big(\zeta^K\big) = \frac{1}{K}\sum_{i=1}^{K}\left[\bar{h}^T\zeta_i + \frac{1}{2}\zeta_i^T\bar{H}\zeta_i\right] + \varkappa_K,$$

where

$$\varkappa_K = \frac{1}{2}\big[\widehat{\Psi}_-(\bar{h}, \bar{H}) - \widehat{\Psi}_+(\bar{h}, \bar{H})\big]$$

and $\widehat{\Psi}_\pm = \widehat{\Psi}_\pm^K$ *are given by* (5.6). *Then the* ϵ*-risk of* $\widehat{G}_{K,\epsilon}(\cdot)$ *goes to* 0 *as* $K \to \infty$.

For proof, see Section B.5 of the supplement paper.

5.2. Numerical illustration, indirect observations

5.2.1. *The problem*

The estimation problem we address in this section is as follows. Our observations are

$$\zeta = Pu + \xi, \tag{5.19}$$

where

- P is a given $d \times m$ matrix, with $m > d$ ("under-determined observations"),
- $u \in \mathbf{R}^m$ is a signal known to belong to a given compact set U,
- $\xi \sim \mathcal{N}(0, \Theta)$ is the observation noise; Θ is positive semidefinite $d \times d$ matrix known to belong to a given convex compact set $\mathcal{V} \subset \mathbf{S}^d_+$.

Our goal is to estimate the energy

$$F(u) = \frac{\|u\|_2^2}{m}$$

of the signal given a single observation (5.19).

In our experiment, the data is specified as follows:

1. We assume that $u \in \mathbf{R}^m$ is a discretization of a smooth function $x(t)$ of continuous argument $t \in [0; 1]$: $u_i = x(\frac{i}{m})$, $1 \le i \le m$, and use in the role of U ellipsoid $\{u \in \mathbf{R}^m : \|Su\|_2^2 \le 1\}$ with S selected to make U a natural discrete-time version of the Sobolev-type ball $\{x : [x(0)]^2 + [x'(0)]^2 + \int_0^1 [x''(t)]^2\,dt \le 1\}$.
2. $d \times m$ matrix P is of the form UDV^T, where U and V are randomly selected $d \times d$ and $m \times m$ orthogonal matrices, and the d diagonal entries in diagonal $d \times m$ matrix D are of the form $\vartheta^{-\frac{i-1}{d-1}}$, $1 \le i \le d$; the "condition number" ϑ of P is a design parameter.
3. The set $\mathcal{V}$ of allowed values of the covariance matrices Θ is the set of all diagonal $d \times d$ matrices with diagonal entries varying in $[0, \sigma^2]$, with the "noise intensity" σ being a design parameter.

5.2.2. *Processing the problem*

Our estimating problem clearly is covered by the setup considered in Section 5.1. In terms of this setup, we specify Θ_* as $\sigma^2 I_d$, V as $\mathcal{V}$, and $M(v)$ as the identity mapping of $\mathbf{S}^d$ onto itself; the mapping $u \mapsto A[u; 1]$ becomes the mapping $u \mapsto Pu$, while the set $\mathcal{Z}$ (which should be a convex compact subset of the set $\{Z \in \mathbf{S}^{d+1}_+ : Z_{d+1,d+1} = 1\}$ containing all matrices of the form $[u; 1][u; 1]^T$, $u \in U$) becomes the set

$$\mathcal{Z} = \big\{Z \in \mathbf{S}^{d+1}_+ : Z_{d+1,d+1} = 1, \operatorname{Tr}\big(Z \operatorname{Diag}\{S^T S, 0\}\big) \le 1\big\}.$$

As suggested by Proposition 5.1, linear in "lifted observation" $\omega = (\zeta, \zeta\zeta^T)$ estimates of $F(u) = \frac{1}{m}\|u\|_2^2$ stem from the optimal solution (h_*, H_*) to the convex optimization problem

$$\mathrm{Opt} = \min_{h,H} \frac{1}{2}\big[\widehat{\Psi}_+(h, H) + \widehat{\Psi}_-(h, H)\big], \tag{5.20}$$

with $\widehat{\Psi}_\pm(\cdot)$ given by (5.6) as applied with $K = 1$. The resulting estimate is

$$\zeta \mapsto h_*^T \zeta + \frac{1}{2}\zeta^T H_* \zeta + \varkappa, \quad \varkappa = \frac{1}{2}\big[\widehat{\Psi}_-(h_*, H_*) - \widehat{\Psi}_+(h_*, H_*)\big] \tag{5.21}$$

and the ϵ-risk of the estimate is (upper-bounded by) Opt.

Problem (5.20) is a well-structured convex-concave saddle point problem and as such is beyond the "immediate scope" of the standard Convex Programming software toolboxes primarily aimed at solving well-structured convex minimization problems. However, applying conic duality, one can easily eliminate in (5.6) the inner maxima over v, Z to arrive at the reformulation which can be solved numerically by CVX (Grant and Boyd [21]), and this is how (5.20) was processed in our experiments.

5.2.3. *Numerical results*

To quantify the performance of the proposed approach, we present, along with the upper risk bounds, simple lower bounds on the best ϵ-risk achievable under the circumstances. The origin of these lower bounds is as follows. Let $w \in U$ with $t(w) = \|Pw\|_2$, and let $\rho = 2\sigma q_{\mathcal{N}}(1-\epsilon)$ where $q_{\mathcal{N}}(\cdot)$ is the standard normal quantile:

$$\mathrm{Prob}_{\xi\sim\mathcal{N}(0,1)}\{\xi \le q_{\mathcal{N}}(p)\} = p \quad \forall p \in (0,1).$$

Then for $\theta(w) = \max[1-\rho/t(w), 0]$, we have $w' := \theta(w)w \in U$, and $\|Pw - Pw'\|_2 \le \rho$. The latter, due to the origin of ρ, implies that there is no test which decides on the hypotheses $u = w$ and $u = w'$ via observation $Pu + \xi$, $\xi \sim \mathcal{N}(0, \sigma^2 I_d)$, with risk $< \epsilon$. As an immediate consequence, the quantity

$$\phi(w) := \frac{1}{2}\bigl[\|w\|_2^2 - \|w'\|_2^2\bigr] = \|w\|_2^2\bigl[1-\theta^2(w)\bigr]/2$$

is a lower bound on the ϵ-risk, on U, of a whatever estimate of $\|u\|_2^2$. We can now try to maximize the resulting lower risk bound over U, thus arriving at the lower bound

$$\mathrm{LwBnd} = \max_{w\in U}\left\{\frac{1}{2}\|w\|_2^2\bigl(1-\theta^2(w)\bigr)\right\}.$$

On a closest inspection, the latter problem is not a convex one, which does not prevent us from building its suboptimal solution.

Note that in our experiments even with fixed design parameters d, m, θ, σ, we still deal with families of estimation problems differing from each other by their "sensing matrices" P; orientation of the system of right singular vectors of P with respect to the axes of U is random, so that these matrices vary essentially from simulation to simulation, which affects significantly the attainable estimation risks. We display in Figure 1 typical results of our experiments. We see that the (theoretical upper bounds on the) ϵ-risks of our estimates, while varying significantly with the parameters of the experiment, all the time stay within a moderate factor from the lower risk bounds.

5.3. Estimation of quadratic functionals of a discrete distribution

In this section, we consider the situation as follows: we are given a $d \times m$ "sensing matrix" A which is stochastic – with columns belonging to the probabilistic simplex $\Delta_d = \{v \in \mathbf{R}^d : v \ge 0, \sum_i v_i = 1\}$, and a nonempty closed subset U of Δ_m, along with a K-repeated observation $\zeta^K = (\zeta_1, \dots, \zeta_K)$ with ζ_k, $1 \le k \le K$, drawn independently across i from the discrete distribution $\mu = Au_*$, where u_* is an unknown probabilistic vector ("signal") known to belong to U. *We*

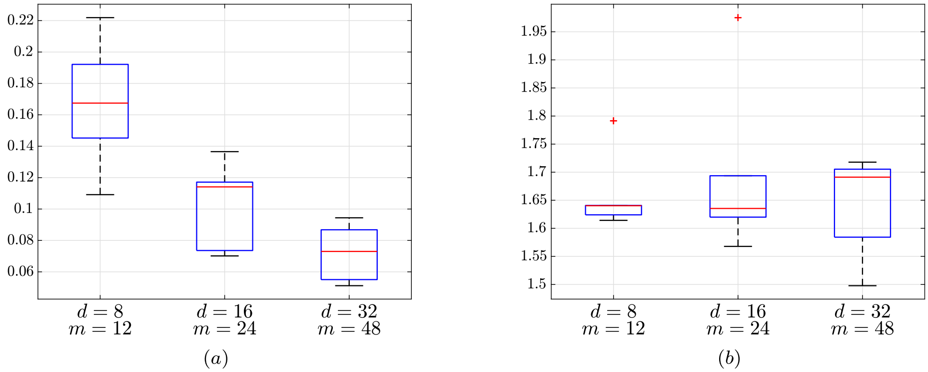


Figure 1. Empirical distribution of the 0.01-risk over 20 random estimation problems, $\sigma = 0.025$. (a): upper risk bound Opt as in (5.20); (b) corresponding suboptimality ratios.

always assume that $K \geq 2$. We treat a discrete distribution on d-point set as a distribution P_μ on the d vertices $e_1, \dots, e_d$ of Δ_d, so that possible values of ζ_i are basic orths $e_1, \dots, e_d$ in $\mathbf{R}^d$ with $\mathrm{Prob}_{\zeta \sim \mu}\{\zeta = e_j\} = \mu_j$. Our goal is to recover from observation ζ^K the value at u_* of a given quadratic form

$$F(u) = u^T Q u + 2q^T u.$$

5.3.1. *Construction*

Observe that for $u \in \Delta_m$, we have $u = [uu^T]\mathbf{1}_m$, where $\mathbf{1}_m$ is the all-ones vector in $\mathbf{R}^m$. This observation allows to rewrite $F(u)$ as a homogeneous quadratic form:

$$F(u) = u^T \bar{Q} u, \ \bar{Q} = Q + \left[q\mathbf{1}_m^T + \mathbf{1}_m q^T\right]. \tag{5.22}$$

Our goal is to construct an estimate $\widehat{G}(\zeta^K)$ of $F(u)$, specifically, estimate of the form

$$\widehat{G}(\zeta^K) = \mathrm{Tr}\big(h\omega[\zeta^K]\big) + \kappa,$$

where $\omega[\zeta^K]$ is the "quadratic lifting" of observation ζ^K (cf. (2.5)):

$$\omega[\zeta^K] = \frac{2}{K(K-1)} \sum_{1 \leq j < j \leq M} \omega_{ij}[\zeta^K], \qquad \omega_{ij}[\zeta^K] = \frac{1}{2}[\zeta_i \zeta_j^T + \zeta_j \zeta_i^T], \quad 1 \leq i < j \leq K,$$

and $h \in \mathbf{S}^d$ and $\kappa \in \mathbf{R}$ are the parameters of the estimate. To this end

- we set $x(u) = uu^T \in X := \{uu^T : u \in U\}$, and specify a convex compact subset $\mathcal{X}$ of the intersection of the "symmetric matrix simplex" $\mathbf{\Delta}^m \subset \mathbf{S}^m$ (see (2.6)) and the cone $\mathbf{S}^m_+$ of positive semidefinite matrices such that $X \subset \mathcal{X} \subset \mathcal{E}_X := \mathbf{S}^m$. We put $\mathcal{F} = \mathcal{E}_F := \mathbf{S}^d$, and $\mathcal{M} = \mathbf{\Delta}^d$, thus $A\mathcal{X}A^T \subset \mathcal{M} \subset \mathcal{E}_M := \mathbf{S}^d$.

- By Proposition 2.2, $\mathcal{F}, \mathcal{M}$ and $\Phi(\cdot;\cdot)$, as defined in (2.7), form a regular data such that setting $M = \lfloor K/2 \rfloor$, for all $u \in U$ and $h \in \mathbf{S}^d$ it holds

$$\begin{gathered}\ln\big(\mathbf{E}_{\zeta\sim P_u}\big\{\exp\{\langle h, \omega[\zeta^K]\rangle\}\big\}\big) \le \Phi_M\big(h; Auu^TA^T\big),\\ \left[\Phi_M(h;Z) = M\ln\left(\sum_{i,j} Z_{ij}\exp\{M^{-1}h_{ij}\}\right) : \mathbf{S}^d \times \mathbf{\Delta}^d \to \mathbf{R}\right],\end{gathered} \tag{5.23}$$

where $\langle h, w\rangle = \mathrm{Tr}(hw)$ is the Frobenius inner product on $\mathbf{S}^d$.

Observe that for $x \in \mathcal{E}_X$, $x \mapsto \mathcal{A}(x) = AxA^T$ is an affine mapping from $\mathcal{X}$ into $\mathcal{M}$, and setting

$$G(x) = \langle \bar{Q}, x\rangle : \mathcal{E}_X \to \mathbf{R},$$

we get a linear functional on $\mathcal{E}_X$ such that

$$G\big(uu^T\big) = \big\langle \bar{Q}, uu^T\big\rangle = F(u).$$

The relation $\Phi(0,z) = 0\ \forall z \in \mathcal{M}$ being obvious, Proposition 2.2 combines with Proposition 3.1 to yield the following result.

Proposition 5.3. *In the situation in question, given $\epsilon \in (0,1)$, let $M = M(K) = \lfloor K/2 \rfloor$, and let*

$$\begin{aligned}
\Psi_+(h,\alpha) &= \max_{x\in\mathcal{X}}\big[\alpha\Phi_M\big(h/\alpha, AxA^T\big) - \mathrm{Tr}(\bar{Q}x)\big] : \mathbf{S}^d \times \{\alpha > 0\} \to \mathbf{R},\\
\Psi_-(h,\alpha) &= \max_{x\in\mathcal{X}}\big[\alpha\Phi_M\big(-h/\alpha, AxA^T\big) + \mathrm{Tr}(\bar{Q}x)\big] : \mathbf{S}^d \times \{\alpha > 0\} \to \mathbf{R},\\
\widehat{\Psi}_+(h) &:= \inf_{\alpha>0}\big\{\Psi_+(h,\alpha) + \alpha\ln(2/\epsilon)\big\}\\
&= \max_{x\in\mathcal{X}}\inf_{\alpha>0}\big[\alpha\Phi_M\big(h/\alpha, AxA^T\big) - \mathrm{Tr}(\bar{Q}x) + \alpha\ln(2/\epsilon)\big]\\
&= \max_{x\in\mathcal{X}}\inf_{\beta>0}\left[\beta\Phi_1\big(h/\beta, AxA^T\big) - \mathrm{Tr}(\bar{Q}x) + \frac{\beta}{M}\ln(2/\epsilon)\right][\beta = M\alpha],\\
\widehat{\Psi}_-(h) &:= \inf_{\alpha>0}\big\{\Psi_-(h,\alpha) + \alpha\ln(2/\epsilon)\big\}\\
&= \max_{x\in\mathcal{X}}\inf_{\alpha>0}\big[\alpha\Phi_M\big(-h/\alpha, AxA^T\big) + \mathrm{Tr}(\bar{Q}x) + \alpha\ln(2/\epsilon)\big]\\
&= \max_{x\in\mathcal{X}}\inf_{\beta>0}\left[\beta\Phi_1\big(-h/\beta, AxA^T\big) + \mathrm{Tr}(\bar{Q}x) + \frac{\beta}{M}\ln(2/\epsilon)\right][\beta = M\alpha].
\end{aligned}$$

The functions $\widehat{\Psi}_\pm$ are real valued and convex on $\mathbf{S}^m$, and every candidate solution $\bar{h}$ to the convex optimization problem

$$\mathrm{Opt} = \min_h\left\{\widehat{\Psi}(h) := \frac{1}{2}\big[\widehat{\Psi}_+(h) + \widehat{\Psi}_-(h)\big]\right\}, \tag{5.24}$$

induces the estimate

$$\widehat{G}_{\bar{h}}(\zeta^K) = \mathrm{Tr}(\bar{h}\omega[\zeta^K]) + \kappa(\bar{h}), \kappa(h) = \frac{\widehat{\Psi}_-(h) - \widehat{\Psi}_+(h)}{2},$$

of the functional of interest (5.22) *via observation* ζ^K *with* ϵ*-risk on* U *not exceeding* $\bar{\rho} = \widehat{\Psi}(\bar{h})$:

$$\forall (u \in U) : \mathrm{Prob}_{\zeta^K \sim P_u^K}\left\{\left|F(u) - \widehat{G}_{\bar{h}}(\zeta^K)\right| > \bar{\rho}\right\} \le \epsilon.$$

5.3.2. *Numerical illustration*

To illustrate the above construction, consider the following problem: we observe independent across $k \le K$ realizations ζ_k of discrete random variable ζ taking values $1, \dots, d$. The distribution $p \in \Delta^d$ of ζ is linearly parameterized by "signal" u which itself is a probability distribution on "discrete square" $\Omega = \Xi \times \Xi$, $\Xi = \{1, \dots, m\}$:

$$p_i = \sum_{1 \le r,s \le m} A_{p,rs} u_{rs}, \quad 1 \le i \le d.$$

Here $A_{i,rs} \ge 0$ are known coefficients such that $\sum_i A_{i,rs} = 1$ for all $(r, s) \in \Omega$. Now, given two sets $I \subset \Xi$ and $J \subset \Xi$, consider the events $\mathcal{I} = I \times \Xi \subset \Omega$ and $\mathcal{J} = \Xi \times J \subset \Omega$. Our objective is to quantify the deviation of these events, the probability distribution on Ω being u, from independence, specifically, to estimate, via observations $\zeta_1, \dots, \zeta_K$, the quantity

$$F_{IJ}(x) = \sum\nolimits_{(r,s) \in I \times J} u_{rs} - \left[\sum\nolimits_{(r,s) \in I \times \Xi} u_{rs}\right]\left[\sum\nolimits_{(r,s) \in \Xi \times J} u_{rs}\right]$$

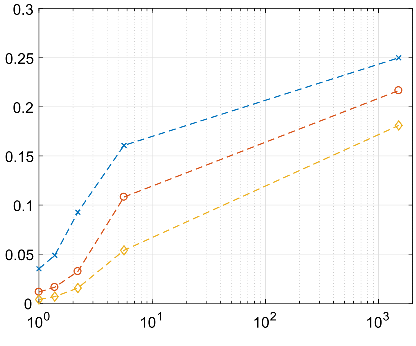
which is a quadratic function of u. In the experiments we report below, this estimation was carried out via a straightforward implementation of the construction presented earlier in this section. Our setup was as follows:

1. We use $d = m^2$. $d \times d$ column-stochastic "sensing matrix" A [9] corresponding to the "mixed-noise observations" Lepski [36], Lepski and Willer [37] is generated according to $A = \theta I_d + (1 - \theta)D$, with column-stochastic $d \times d$ matrix D, $\theta \in [0, 1]$ being our control parameter. D was selected at random, by normalizing columns of a $d \times d$ matrix with independent entries drawn from the uniform distribution on $[0, 1]$;
2. We set

$$\mathcal{X} = \left\{x \in \mathbf{S}^d : x_{rs,r's'} \ge 0 \; \forall r, s, r', s' \le m, x \succeq 0, \sum_{1 \le r,s,r',s' \le m} x_{rs,r's'} = 1\right\}$$

   which is the simplest convex outer approximation of the set $\{uu^T : u \in \Delta_d\}$.
3. We use $I = J = \{1, 2, 3\} \subset \Xi = \{1, 2, \dots, 8\}$, $\epsilon = 0.01$, $m = 8$ (i.e., $d = 64$).

[9]we identify the $m \times m$ "discrete square" Ω with $\{1, \dots, d\}$, which allows to treat a probability distribution u on Ω as a vector from Δ_d.



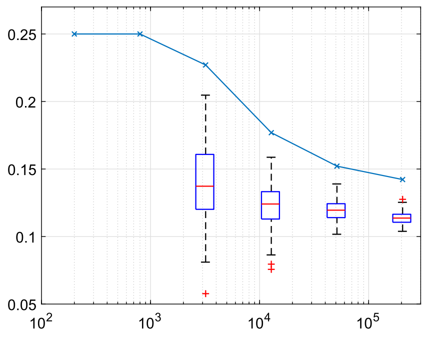


Figure 2. Estimation of "independence defect." (a): Upper risk bound (value Opt in (5.24)) of linear estimate as a function of condition number cond(A); data for $K = 2 \cdot 10^3, 2 \cdot 10^4$ and $2 \cdot 10^5$. (b): risk of linear estimation as function of K along with boxplots of empirical error distributions for 100 simulations ($\theta = 0.1$, cond$(A) = 39.2$).

We present in Figure 2 the results of experiments for θ taking values in $\{0.00, 0.25, 0.50, 0, 75, 1.00\}$. Other things being equal, the smaller θ, the larger is the condition number cond(A) of the sensing matrix, and thus the larger is the (upper bound on the) risk of our estimate – the optimal value of (5.24). Note that the variation of F_{IJ} over X is exactly $1/2$, so the maximal risk is $\leq 1/4$. It is worthy to note that simple (if compared, e.g., to much more involved results of Houdré and Reynaud-Bouret [23]) bounds in Proposition 2.2 for Laplace functional of order-2 U-statistics distribution result in fairly good approximations of the risk of our estimate (cf. the boxplots of empirical distributions of the estimation error in the right plot of Figure 2).

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Supplementary Material

Supplement A: Numerical illustration for Section 4 and proofs (DOI: 10.3150/20-BEJ1200SUPP; .pdf). In the supplement, we provide numerical illustration for Section 4 and full proofs of the results appearing in the paper.

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