Optimization Bias in Covariance Estimation: Effect of Model Misspecification

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Section 1

Problem Formulation

Overview

Given a $p \times n$ data matrix Y,

- The true (unknown) model is defined as

$$Y_{p\times n} = B_{p\times q} X_{q\times n} + \epsilon_{p\times n} \tag{1}$$

- The true covariance matrix Σ is:

$$\Sigma = \mathscr{B}\Lambda\mathscr{B}^\top + \gamma^2 I, \tag{2}$$

  - Λ: $q \times q$ diagonal matrix, eigenvalues of $BB^\top$
  - $\mathscr{B}$: $p \times q$ matrix of corresponding eigenvectors
  - γ: $E(\epsilon^\top \epsilon) = \gamma^2 I$

We don't know $q \Rightarrow$ We choose a K.

$K = 1$

Assume the true number of factors $q > 1$, and we choose the estimate $K = 1$. The population covariance matrix that we *believe* is

$$\Sigma^* = \sigma_p^2 bb^\top + \gamma^2 I, \tag{3}$$

where σ_p^2 is the largest eigenvalue of $bb^\top$. This motivates the estimated covariance matrix as

$$\hat{\Sigma} = s^2 hh^\top + \hat{\gamma}^2 I. \tag{4}$$

Note: we use * to denote our belief and $\hat{}$ to denote the estimate.

Notations & Covariance Matrix Models

q	True number of spikes
K	Estimated number of spikes
$\mathscr{B}$	Eigenvectors of $BB^\top$
b	First column of $\mathscr{B}$, normalized to length 1
h	Leading eigenvector of $\hat{\Sigma} = YY^\top/n$
$s_{i,p}^2$	The i-th eigenvalue of $\hat{\Sigma} = YY^\top/n$
λ_i^2	The $i-$th eigenvalue of $L = Y^\top Y/p$

Table: Notations

Σ	True (unknown) population covariance matrix
Σ^*	Covariance matrix when we choose $K = 1$; $\Sigma^* = \sigma_p^2 bb^\top + \gamma^2 I$
$\hat{\Sigma}$	Sample covariance matrix based on $K = 1$; $\hat{\Sigma} = s^2 hh^\top + \hat{\gamma}^2 I$

Table: Comparison Table

Section 2

$K = 1$ Recipe

$h_\sharp$ Construction

Recipe:

$$h_\sharp = \frac{1}{D}(\psi^2 h + N z_{\perp h}), \tag{5}$$

where

$$z_{\perp h} = \frac{z - z_h}{|z - z_h|}$$

with

$$z_h = \langle h, z \rangle h$$

.

- z: the direction that we want to study
- z_h: the projection of z onto h
- $z_{\perp h}$: the unit vector in the direction of the component of z that's orthogonal to h
- D: a normalizing constant
- ψ^2: signal-to-noise ratio

Details in $h_\sharp$

Define

$$\psi^2 = \frac{s_{1,p}^2 - l_p^2}{s_{1,p}^2}, \text{ with } l_p^2 \text{ be average non-zero bulk eigenvalues.}$$
$$N = \frac{\langle h, z\rangle - \psi^2 \langle h, z\rangle}{\sqrt{1 - \langle h, z\rangle^2}}, \tag{6}$$
$$D = \sqrt{\psi^4 + N^2}$$

- ψ^2: signal-to-noise ratio. ψ^2 is high – put more weight on h
- N: the correction strength in the direction orthogonal to h, scaled by the noise level $(1 - \psi^2)$ and alignment between h and z. N is high – need to pull back by adding more weight on $z_{\perp h}$.

Section 3

Optimization Bias

$\mathcal{E}_p(h)$

For $z \in \mathbb{R}^p$ with $|z| = 1$, the *true* quadratic optimization function is defined as:

$$\mathcal{E}_p(h) = \frac{\mathscr{B}^\top z - \mathscr{B}^\top \mathscr{H} \mathscr{H}^\top z}{\sqrt{1 - \langle \mathscr{H}, z \rangle^2}} \tag{7}$$

Connecting to minimum variance problem:
The expected out-of-sample variance $V_p^2 = \langle \hat{w}, \Sigma \hat{w} \rangle$ can be written as

$$V_p^2 = \frac{|\Lambda_p \mathcal{E}_p(\mathscr{H})|^2}{p|z - z_{\mathscr{H}}|^2} + O(1/p), \tag{8}$$

so $V_p^2 \to 0 \iff |\mathcal{E}_p(\mathscr{H})| \to 0$.

$\mathscr{E}_p^*(h)$

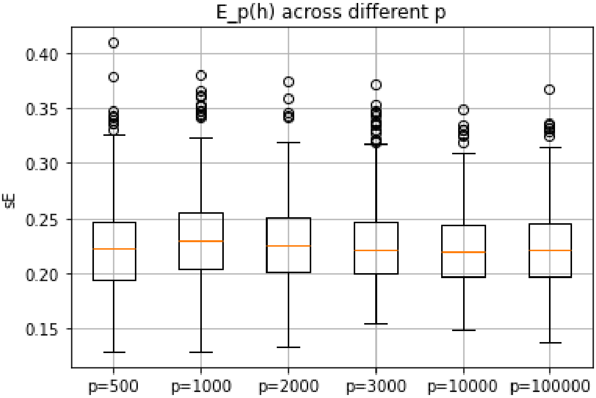
We *believe* the optimization bias is

$$\mathscr{E}_p^*(h) = \frac{\langle b, z\rangle - \langle b, h\rangle\langle h, z\rangle}{\sqrt{1 - \langle h, z\rangle^2}}. \tag{9}$$

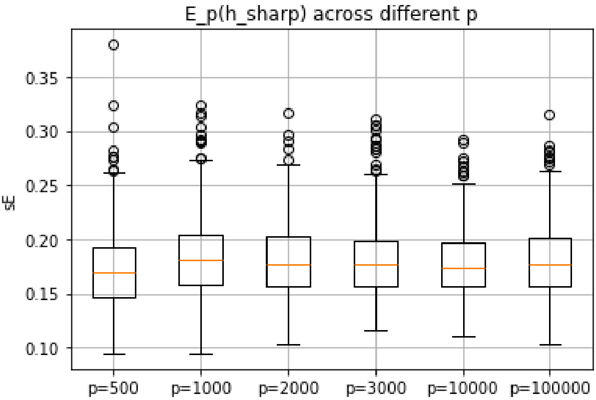
Note it is the first component of the true $\mathscr{E}_p(h)$ (by writing $B = (\beta_1, \beta_2, \cdots, \beta_q)$ and $b = \beta_1/|\beta_1|$).

When $q = K = 1$, $\mathscr{E}_p^*(h) \to 0$.

$|E_p^*(h)|$ v.s. p $(q = 7)$


E_p(h) across different p
0.40
0.35
0.30
0.25
0.20
0.15
SE
p=500
p=1000
p=2000
p=3000
p=10000
p=100000

$|E_p^*(h_\sharp)|$ v.s. p $(q = 7)$



Section 4

Main Theorem

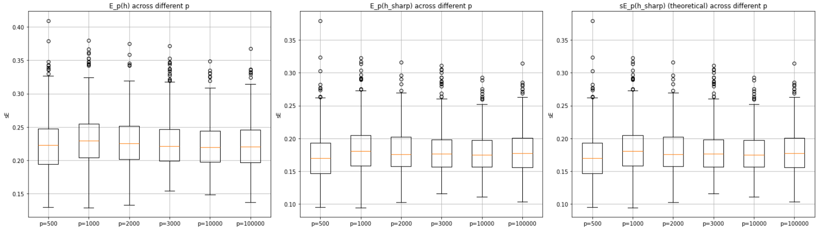
Theorem

Theorem

For $\psi^2 = \frac{s_p^2 - l_p^2}{s_p^2}$, where l_p^2 is the average non-zero eigenvalues, we have the following results:

1. $\mathscr{E}_p^*(h_\sharp) = \frac{\psi^2\langle b,z\rangle - \langle h,b\rangle\langle h,z\rangle}{\sqrt{\psi^4 + (1-2\psi^2)\langle h,z\rangle^2}}$.
2. *When* $K = 1 = q$, $\mathscr{E}_p^*(h_\sharp) \to 0$
3. *When* $K = 1 < q$, $\mathscr{E}_p^*(h_\sharp) \not\to 0$.

$|E_p^*|$ v.s. p $(q = 7)$


E_p(h) across different p
E_p(h_sharp) across different p
sE_p(h_sharp) (theoretical) across different p
sE
p=500
p=1000
p=2000
p=3000
p=10000
p=100000

$|E_p^*|$ v.s. q I

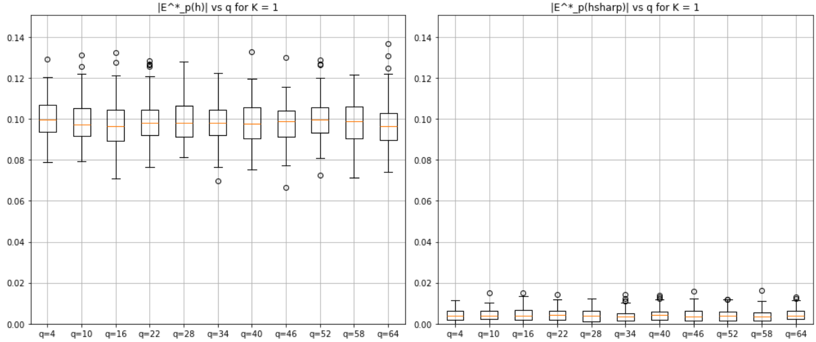


Figure: 1 spiked factor volatility in B construction. B: [market style block] $\times$ factor return matrix

$|E_p^*|$ v.s. q II

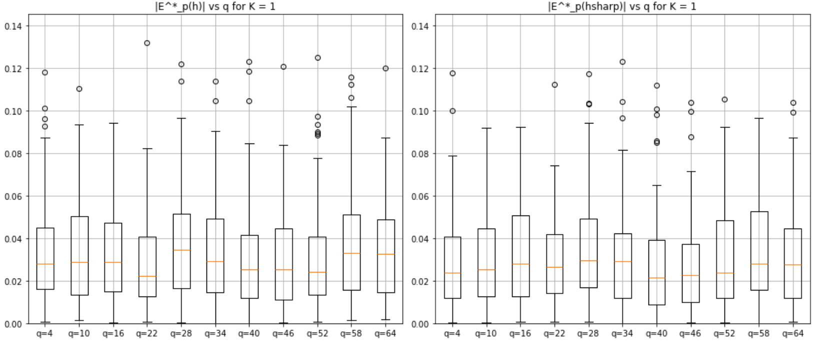


Figure: 2 spiked factor volatilities in B construction. B: [market style block] $\times$ factor return matrix

$|E_p^*|$ v.s. q for Different Factor Volatilities I

Note: the first two diagonal elements of factor vol matrix is 16 and 8, the remains are randomly drawed integers between 1 and M.

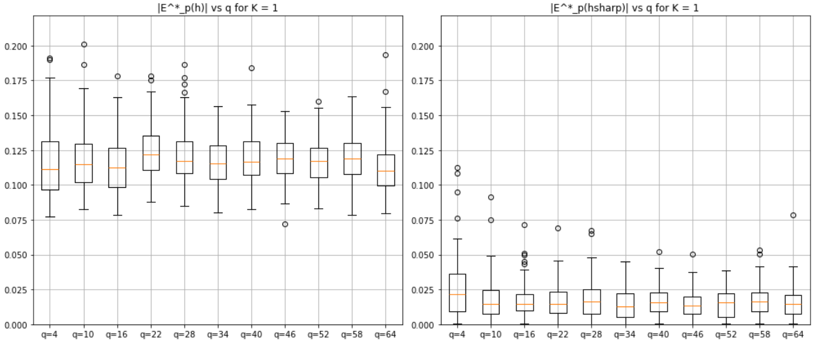


Figure: $M = 25$

$|E_p^*|$ v.s. q for Different Factor Volatilities II

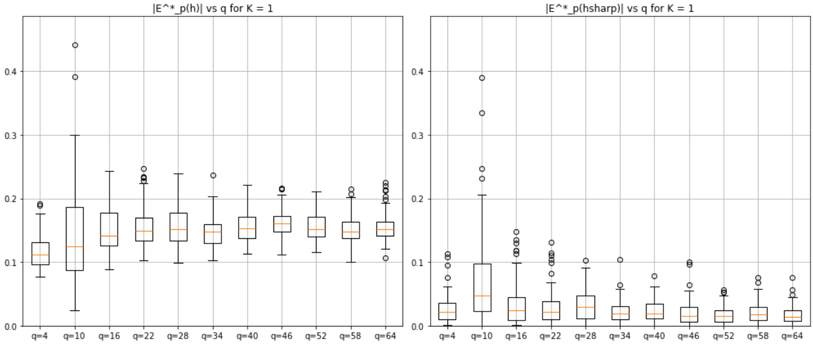


Figure: $M = 50$

$|E_p^*|$ v.s. q for Different Factor Volatilities III

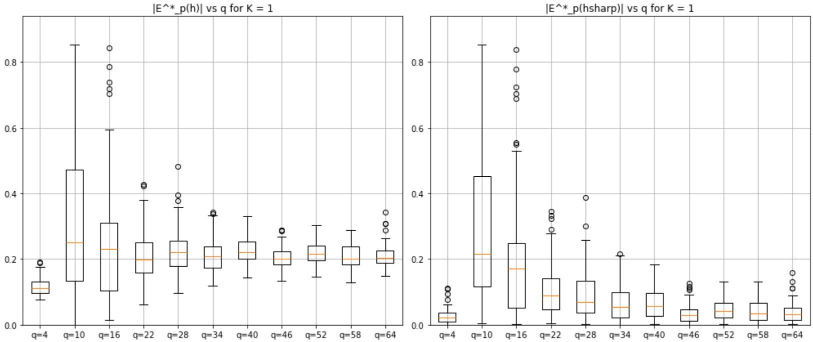


Figure: $M = 75$

$|E_p^*|$ v.s. q for Different Factor Volatilities IV

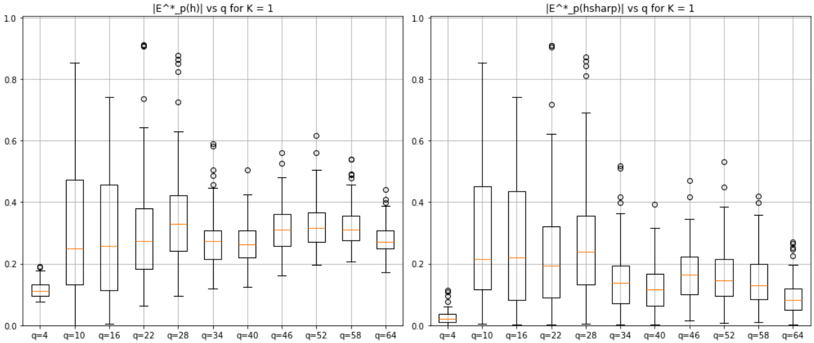


Figure: $M = 100$

Section 5

Appendix

$q = 1$ Asymptotics

If $K = q = 1$, we have

1. $\lim_{p\uparrow\infty} |\langle h, b\rangle^2 - \psi^2| = 0$ for $\psi^2 = 1 - \kappa_p^2 s_{1,p}^{-2}$, where $\kappa_p^2 = \frac{\sum_{j>q} s_{j,p}^2}{n-q}$
2. $\lim_{p\uparrow\infty} |\langle h, z\rangle - \langle h, b\rangle\langle b, z\rangle| = 0$

As $p \to \infty$,

$$\begin{aligned}\langle b, z\rangle - \langle b, h\rangle\langle h, z\rangle &= \langle b, z\rangle - \langle b, h\rangle\langle h, b\rangle\langle b, z\rangle \\ &= \langle b, z\rangle(1 - \langle b, h\rangle\langle h, b\rangle) \neq 0\end{aligned} \tag{10}$$

$\mathscr{E}_p^*(h_\sharp)$

Recall $\mathscr{E}_p^*(h_\sharp) = \mathscr{E}_p^*(h_z t_\sharp)$. Define $\tilde{\mathscr{E}}_p(\cdot) : t \mapsto \mathscr{E}_p^*(h_z t)$. Claim: $t \mapsto \tilde{\mathscr{E}}_p(t)$ is continuous in $\mathbb{R}$.

1. $\langle h_z t, z\rangle < 1$
2. $\langle b, z\rangle - \langle b, h_z t\rangle\langle h_z t, z\rangle = \langle b, z\rangle - t^2\langle b, h_z\rangle\langle h_z, z\rangle$ is continuous w.r.t t.

Now we have for $1 = K = q$:

$$\left.\begin{aligned} &\tilde{\mathscr{E}}_p(t) \textit{ is continuous} \\ &\tilde{\mathscr{E}}_p(t_\sharp) = \tilde{\mathscr{E}}_p(t_\sharp - t_* + t_*) \\ &\tilde{\mathscr{E}}_p(t_*) = \mathscr{E}_p^*(h_z t_*) = 0 \\ &|t_\sharp - t_*| \to 0 \end{aligned}\right\} \Rightarrow \mathscr{E}_p^*(h_\sharp) \to 0. \tag{11}$$

When $1 = K < q$, $|t_\sharp - t_*| \not\to 0$.

$\mathscr{E}_p^*(h_\sharp)$ (Continued)

Let $D = \sqrt{\psi^4 + \frac{(\langle h,z\rangle - \psi^2\langle h,z\rangle)^2}{1-\langle h,z\rangle^2}}$ and $N = \frac{\langle h,z\rangle - \psi^2\langle h,z\rangle}{\sqrt{1-\langle h,z\rangle^2}}$. Note that

1. $\langle h_\sharp, z\rangle = \frac{\langle h,z\rangle}{D}$
2. $\langle h_\sharp, b\rangle = \frac{\psi^2\langle h,b\rangle + (1-\psi^2)\langle h,z\rangle\langle z,b\rangle - \langle h,b\rangle\langle h,z\rangle^2}{D(1-\langle h,z\rangle^2)}$

we have

$$\begin{aligned}\mathscr{E}_p^*(h_\sharp) &= \frac{D\langle b,z\rangle}{\sqrt{D^2-\langle h,z\rangle^2}} - \frac{\psi^2\langle h,b\rangle\langle h,z\rangle + (1-\psi^2)\langle h,z\rangle^2\langle b,z\rangle - \langle h,z\rangle^3\langle h,b\rangle}{D(1-\langle h,z\rangle^2)\sqrt{D^2-\langle h,z\rangle^2}} \\ &= \frac{(\psi^2-\langle h,z\rangle^2)(\psi^2\langle b,z\rangle - \langle h,b\rangle\langle h,z\rangle)}{D(1-\langle h,z\rangle^2)\sqrt{D^2-\langle h,z\rangle^2}} \\ &= \frac{\psi^2\langle b,z\rangle - \langle h,b\rangle\langle h,z\rangle}{\sqrt{\psi^4+(1-2\psi^2)\langle h,z\rangle^2}}\end{aligned} \tag{12}$$

ϕ^2 I

Denote the columns of B be $\beta_1, \beta_2, \cdots, \beta_q$, with each $\beta_i \in \mathbb{R}^p$. Define

$$
\begin{aligned}
D_1 &= \begin{pmatrix} (\beta_1^\top b)(b^\top \beta_1) - \beta_1^\top \beta_1 & \cdots & (\beta_1^\top b)(b^\top \beta_q) - \beta_1^\top \beta_q \\ \vdots & \ddots & \vdots \\ (\beta_q^\top b)(b^\top \beta_1) - \beta_q^\top \beta_1 & \cdots & (\beta_q^\top b)(b^\top \beta_q) - \beta_q^\top \beta_q \end{pmatrix}, \\
D_2 &= \begin{pmatrix} (\beta_1^\top b)\beta_1 - \beta_1^\top & \cdots & (\beta_1^\top b)\beta_q - \beta_1^\top \\ \vdots & \ddots & \vdots \\ (\beta_q^\top b)\beta_1 - \beta_q^\top & \cdots & (\beta_q^\top b)\beta_q - \beta_q^\top \end{pmatrix}, \\
D_3 &= \begin{pmatrix} (bb^\top - 1)\beta_1 & \cdots & (bb^\top - 1)\beta_q \end{pmatrix}
\end{aligned} \tag{13}
$$

And

$$
M_p = \frac{\epsilon^\top bb^\top \epsilon}{p}, \; \Gamma_p = \frac{\epsilon^\top \epsilon}{p}, \; N_p = \frac{X^\top D_1 X + \epsilon^\top D_2 X + X^\top D_3 \epsilon}{p}. \tag{14}
$$

ϕ^2 II

Let $\omega = Y^\top h/(s_{1,p}\sqrt{n})$ denote the leading eigenvector of the dual covariance matrix L with eigenvalue λ_1^2, and $\mathcal{W} = \omega\sqrt{p/(ns_{1,p}^2)}$, then we have

Theorem

1. $\langle h, b\rangle^2 = \omega^\top(L + M_p - \Gamma_p + N_p)\omega/\lambda_1^2 = 1 + \omega^\top(M_p - \Gamma_p + N_p)\omega/\lambda_1^2$
2. *Let* $\phi^2 = \psi^2 + \mathcal{W}^\top(N_p + \frac{n\kappa_p^2}{p}I - \Gamma_p)\mathcal{W}$, *then* $|\langle h, b\rangle^2 - \phi^2| \to 0$.

- When true $q = 1$, the signal space effectively reduces to the single axis spanned by b. The largest eigenvalue is well separated from any noise directions, so the sample covariance matrix naturally aligns h with b.
- When $q > 1$, the signal space becomes multi-dimensional. The estimated h will always pick up contributions from other spikes. Consequently, $\langle h, b\rangle^2$ cannot match the single-spike formula ψ^2.

$1 = K < q$ Asymptotics

Denote $Z_p = bb^\top BX + bb^\top \epsilon$, we have

$$\begin{aligned} |\langle h, z\rangle - \langle h, b\rangle\langle b, z\rangle| &= |h^\top z - (bb^\top h)^\top z| \\ &= \frac{1}{\sqrt{p}} \left| \mathcal{W}^\top X^\top B^\top z + \mathcal{W}^\top \epsilon^\top z - \mathcal{W}^\top Z_p^\top z \right| \\ &= \frac{1}{\sqrt{p}} \left| \mathcal{W}^\top \epsilon^\top (I - bb^\top) z + \mathcal{W}^\top X^\top B^\top (I - bb^\top) z \right| \end{aligned} \tag{15}$$

Since $\overline{\lim}_{p\to\infty} |\mathcal{W}^\top| < \infty$ and $|\epsilon^\top (I - bb^\top) z| / \sqrt{p} \to 0$, we have

Lemma

1. $|\langle h, z\rangle - \langle h, b\rangle\langle b, z\rangle| \sim \frac{|\mathcal{W}^\top X^\top B^\top (I - bb^\top) z|}{\sqrt{p}}$
2. $\left| \langle h, b\rangle \mathscr{E}_p^*(h) - \frac{\langle h,z\rangle - \phi^2 \langle h,z\rangle}{\sqrt{1-\langle h,z\rangle^2}} \right| \sim \frac{|\mathcal{W}^\top X^\top B^\top (I - bb^\top) z|}{\sqrt{p(1-\langle h,z\rangle^2)}} > 0.$

Section 6

Plots

$|E_p^*|$ v.s. q I

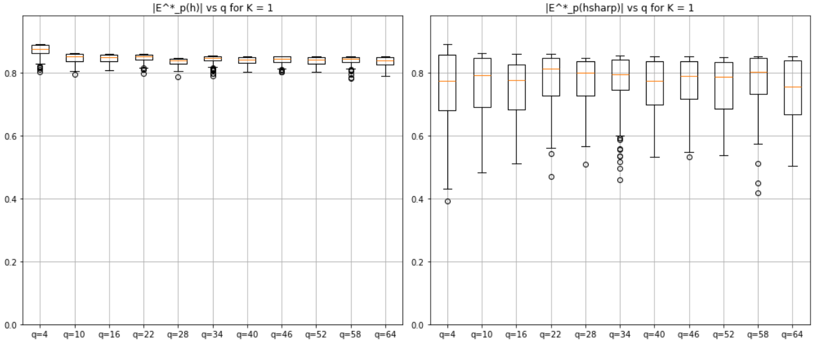


Figure: Factor Vol $= 1$

$|E_p^*|$ v.s. q II

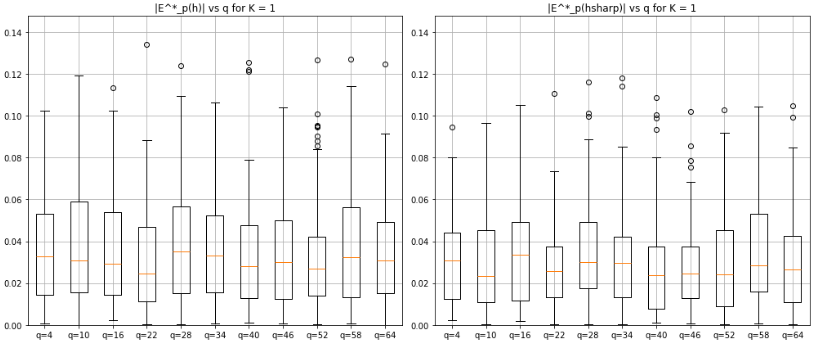
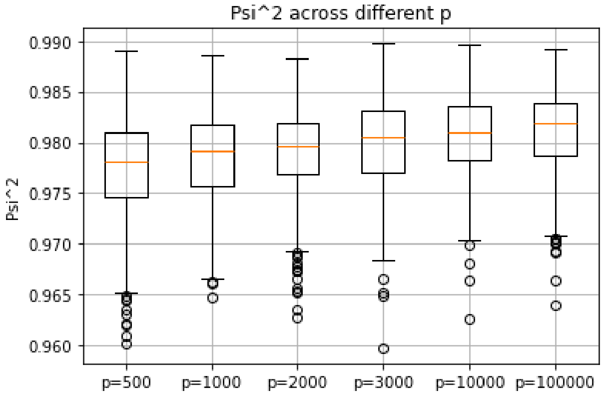
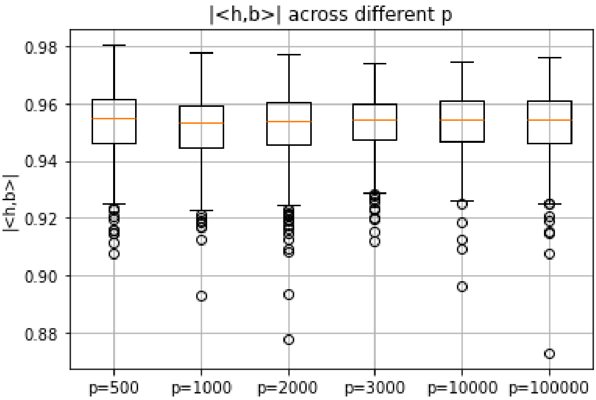


Figure: Factor Vol = 20

ψ^2 v.s. p


Psi^2 across different p
Psi^2
0.990
0.985
0.980
0.975
0.970
0.965
0.960
p=500
p=1000
p=2000
p=3000
p=10000
p=100000

$|\langle h, b \rangle|$ v.s. p



$\langle h, z\rangle^2$ v.s. p