Inrobin
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Experiment one:

Calibration of the Hyperparameters to assess performances of the KTA

Set the notation of this experiment as follows:
Ω_{test} - the set with M_{test} parameters
Ω_{true} - the set with M_{true} parameters
Let $\Psi_{test}^{(i)}$ be an ith parameter from Ω_{test}
Let $\Psi_{true}^{(j)}$ be an jth parameter from Ω_{true}
$k(\cdot, \cdot; \Psi)$ a kernel function from parameterized by the parameter Ψ, $k : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$
Let $\mathbf{t}$ be a $1 \times N$ vector of real numbers
$\mathbf{K}_{true} = k(\mathbf{t}, \mathbf{t}; \Psi = \Psi_{true})$
$\mathbf{K}_{test} = k(\mathbf{t}, \mathbf{t}; \Psi = \Psi_{test})$
$i \in \Big\{1, \cdots, M_{test}\Big\}$, $j \in \Big\{1, \cdots, M_{true}\Big\}$
$\Psi_{test}^{(i)} = \Omega_{true}[i]$
$A(K1, K2) := 2 - \left\| \frac{K_1}{\|K_1\|_F} - \frac{K_2}{\|K_2\|_F} \right\|_F$
$m \in 1, \cdots, M$

Algorithm 1: Algorithm

Input: Define $k, \Omega_{true}, \Omega_{test}, \mathbf{t}$
Set i, j, m

1. Evaluate the Gram Matrix $\mathbf{K}_{(true,j)} = k(\mathbf{t}, \mathbf{t}; \Psi_{(true,j)})$ parametrized by the jth parameter from Ω_{true}
2. Simulate $\mathbf{y}^{(m)} \sim \mathcal{N}(0, \mathbf{K}_{(true,j)})$ be an N dimensional vector
3. Compute the sample covariance matrix given by $\mathbf{S}_{N\times N}^{(m)} = \mathbf{y}^{(m)T}\mathbf{y}^{(m)}$
4. Evaluate the Gram Matrix $\mathbf{K}_{(test,i)} = k(\mathbf{t}, \mathbf{t}; \Psi_{(test,i)})$ parametrized by the ith parameter from Ω_{test}
5. Compute the CKTA given by $a_{j,i,m} = A(\mathbf{S}_{N\times N}^{(m)}, \mathbf{K}_{(test,i)})$

Algorithm 2: Algorithm

Input: Define $k, \Omega_{true}, \Omega_{test}, \mathbf{t}$

for ($j = 1 : M_{true}$) {

  Evaluate $\mathbf{K}_{(true,j)} = k(\mathbf{t}, \mathbf{t}; \Psi_{(true,j)})$

  for ($m = 1 : M$) {

    Simulate $\mathbf{y}^{(m)}_{1\times N} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_{(true,j)})$

    Compute $\mathbf{S}^{(m)}_{N\times N} = \mathbf{y}^{(m)T}\mathbf{y}^{(m)}$

    for ($i = 1 : M_{test}$) {

      Evaluate the Gram Matrix $\mathbf{K}_{(test,i)} = k(\mathbf{t}, \mathbf{t}; \Psi_{(test,i)})$ parametrized by the ith parameter from Ω_{test}

      Compute the CKTA given by $a_{j,i,m} = A(\mathbf{S}^{(m)}_{N\times N}, \mathbf{K}_{(test,i)})$

DOROTA:

way of presenting

which one do we want

difference psi? check together

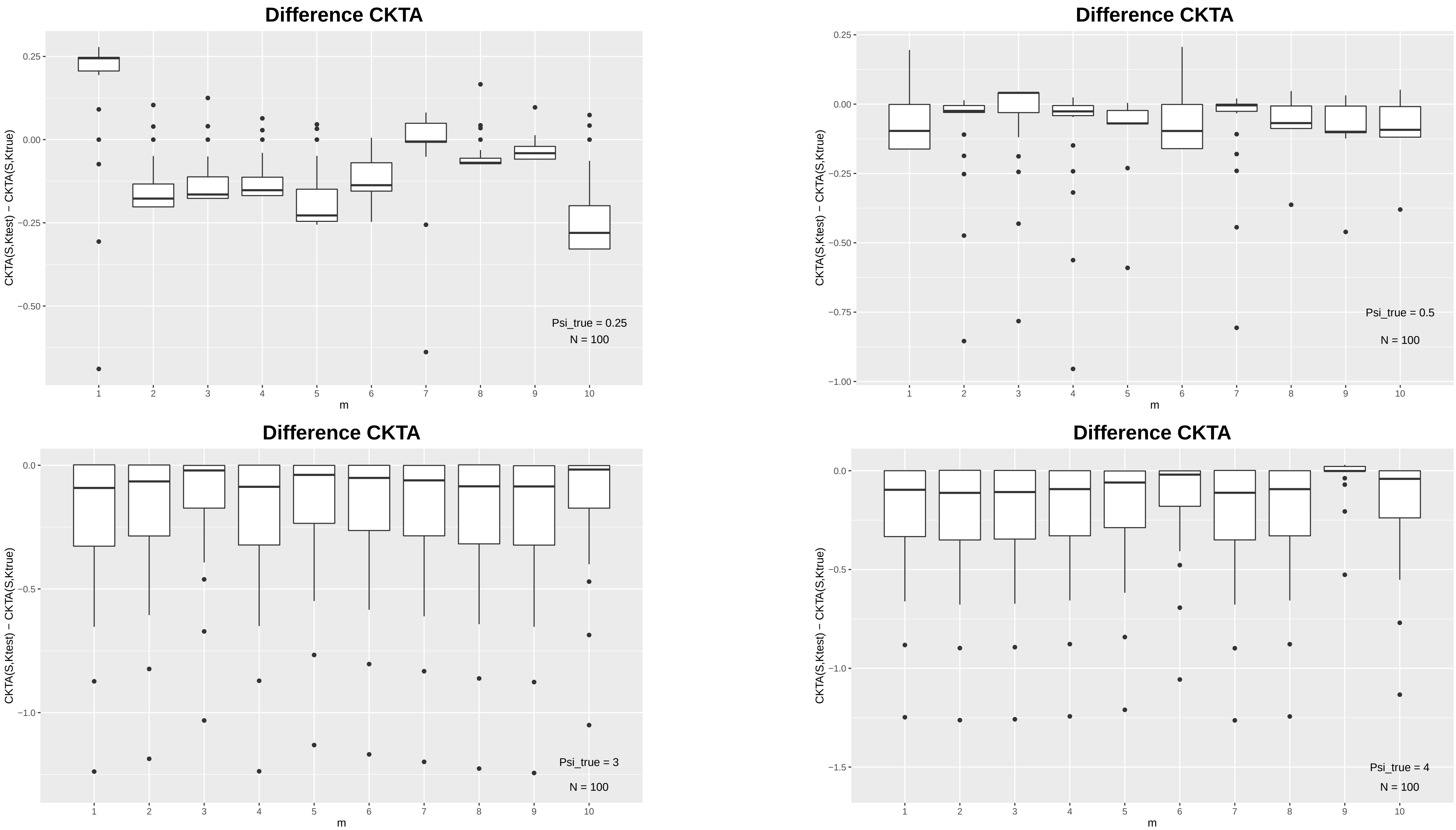


Figure 1: Boxplot of CKTA differences with $m = 10$, $N = 100$. From top left to bottom right $\Psi_{true} = 0.25, 0.5, 3, 4$

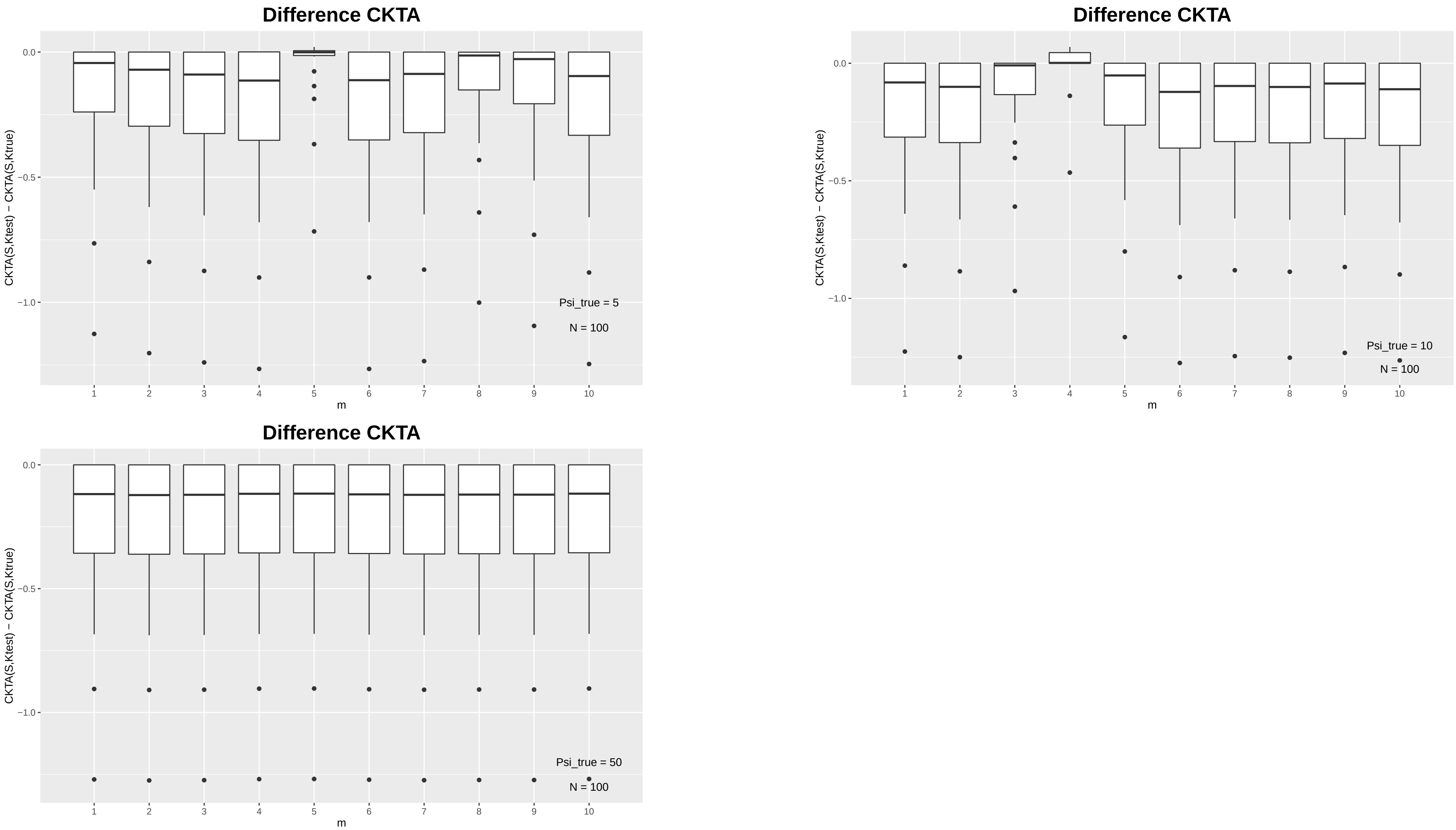
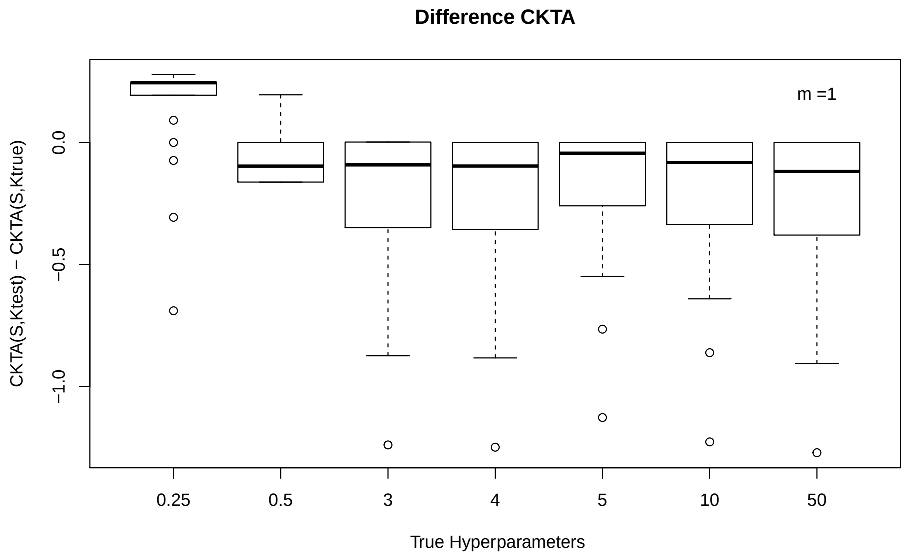
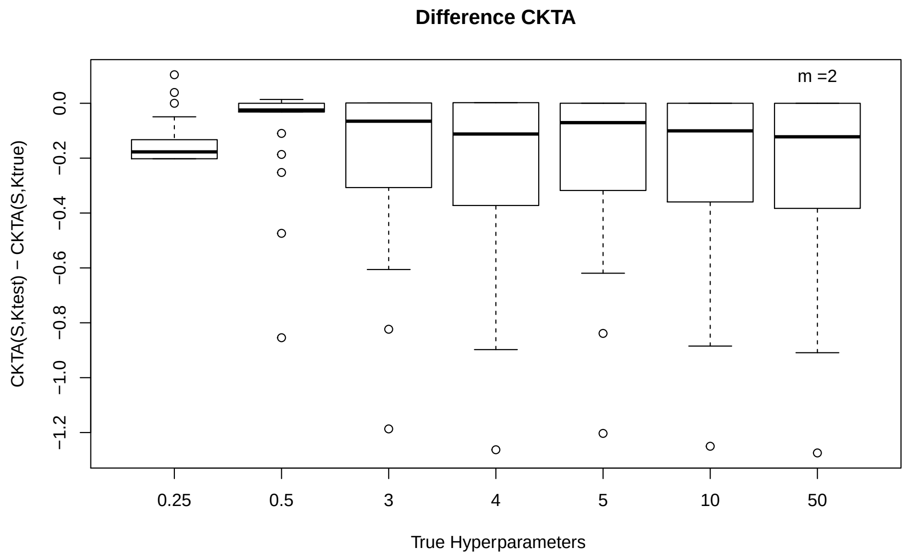
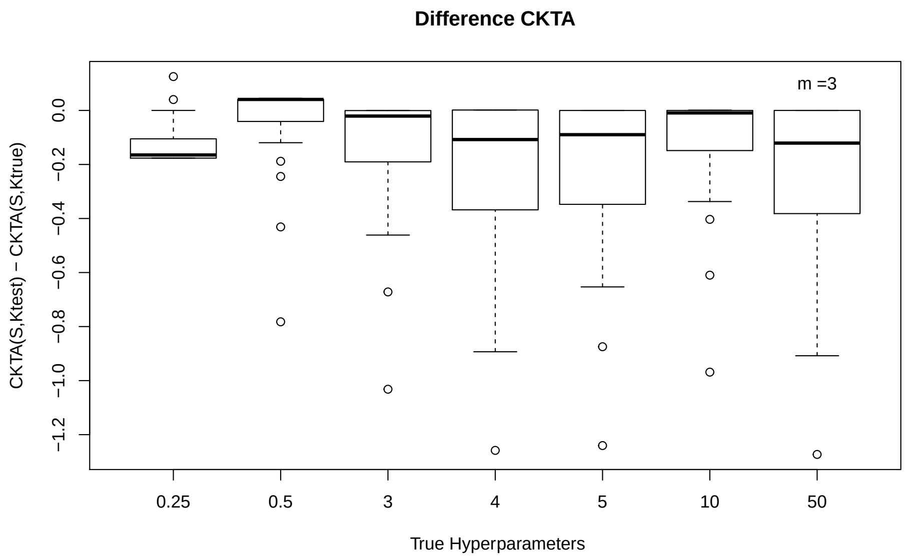
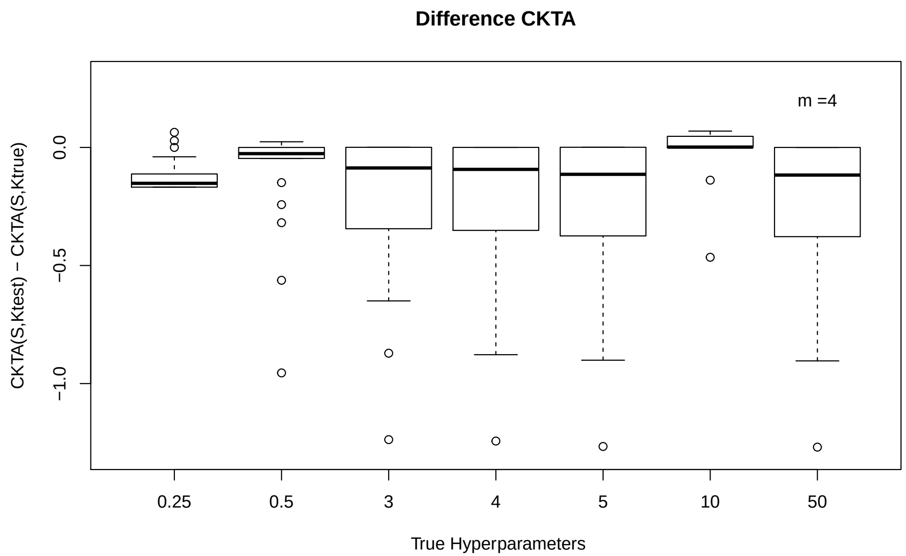


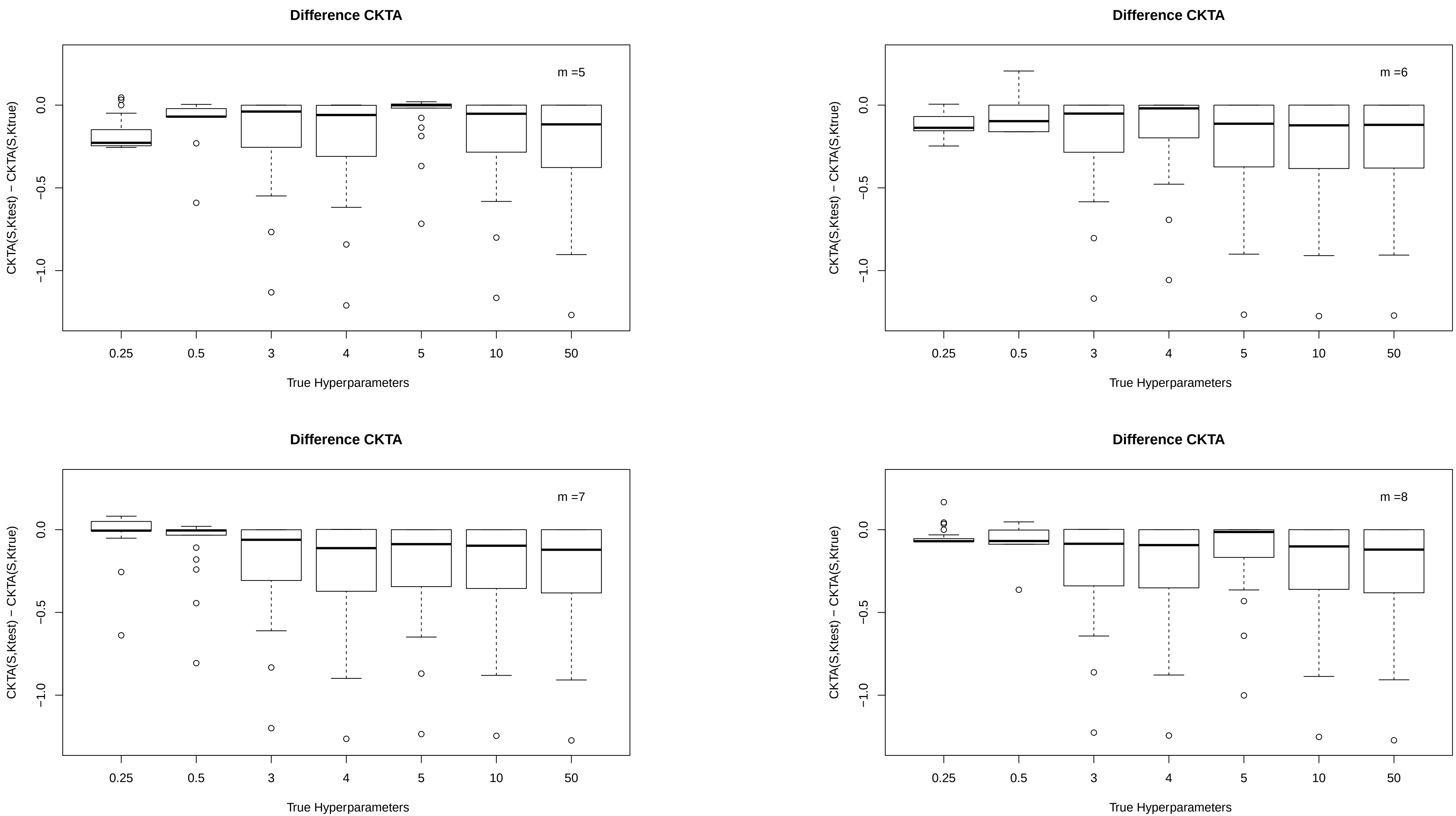
Figure 2: Boxplot of CKTA differences with $m = 10$, $N = 100$. From top left to bottom left $\Psi_{true} = 5, 10, 50$


Difference CKTA
m =1
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.5
−1.0
0.25
0.5
3
4
5
10
50
True Hyperparameters

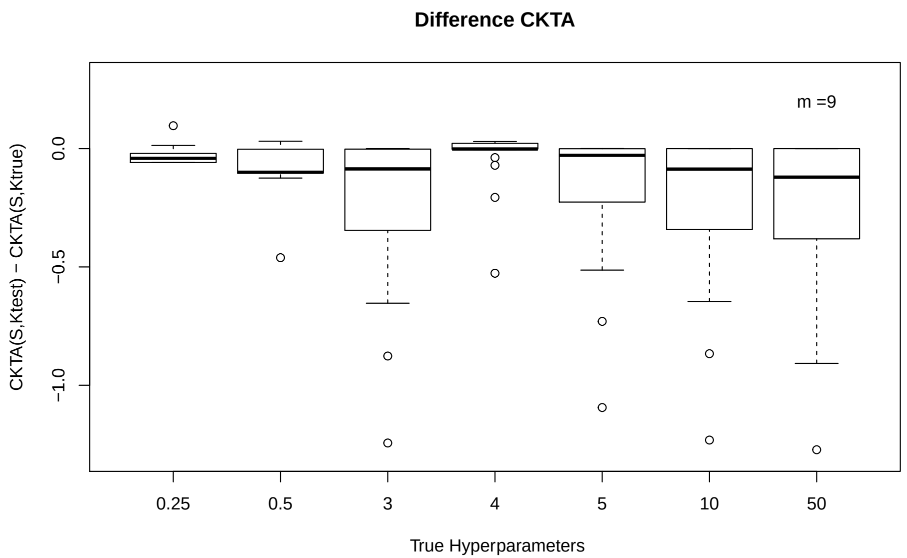

Difference CKTA
m =2
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
0.25
0.5
3
4
5
10
50
True Hyperparameters

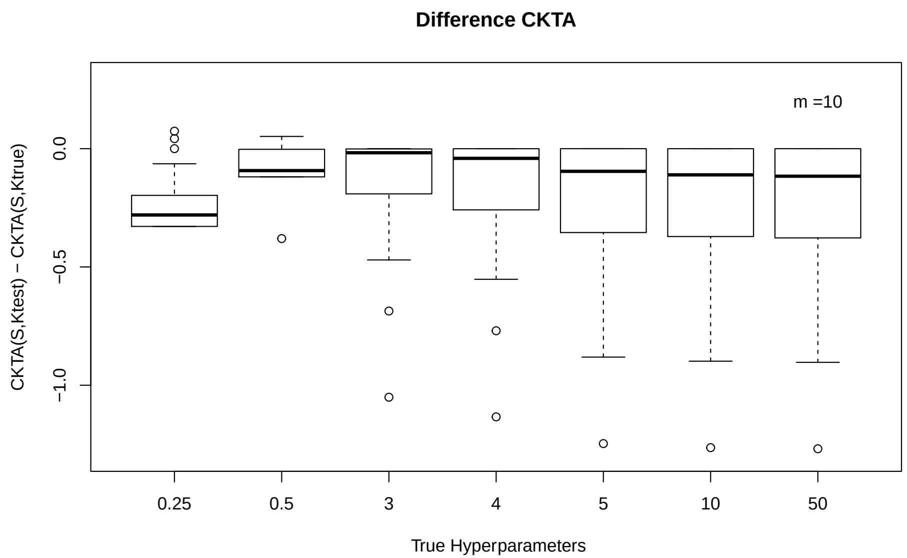

Difference CKTA
m =3
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
0.25
0.5
3
4
5
10
50
True Hyperparameters


Difference CKTA
m =4
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.5
−1.0
0.25
0.5
3
4
5
10
50
True Hyperparameters



Difference CKTA
m =5
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.5
−1.0
0.25
0.5
3
4
5
10
50
True Hyperparameters
Difference CKTA
m =6
Difference CKTA
m =7
Difference CKTA
m =8


Difference CKTA
m =9
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.5
−1.0
0.25
0.5
3
4
5
10
50
True Hyperparameters


Difference CKTA
m =10
CKTA(S,Ktest) − CKTA(S,Ktrue)
0.0
−0.5
−1.0
0.25
0.5
3
4
5
10
50
True Hyperparameters