

Posterior Expectation & Minimum Distance Estimation over Adaptive Histograms from randomized Priority Queues on Statistical Regular Pavings

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Massive Metric Data Streams

Air Traffic Examples (Teng, Kuhn and S., *Jnl. Aerospace Comp., Inf. & Commun.*, [acc.] 2012)

Synthetic Examples (Teng, Harlow, Lee and S., *ACM Trans. Mod. & Comp. Sim.*, [r. 2] 2012)

Regular Pavings (RPs)

Statistical Regular Pavings (SRPs)

Adaptive Histograms

S.E.B. Priority Queue

Arithmetic on SRPs

Posterior Expectation over Histograms in $\mathbb{S}_{0:\infty}$

Examples - good, bad and ugly

Setting up MDE

An Example

Minimum Distance Estimation

Conclusions and References

Massive Metric Data Streams – Introduction

- ▶ A massive metric data stream is:

$$\dots, X_{-3}, X_{-2}, X_{-1}, X_0, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_n, X_{n+1}, \dots \sim F, \quad X_i \in \mathbb{R}^d.$$

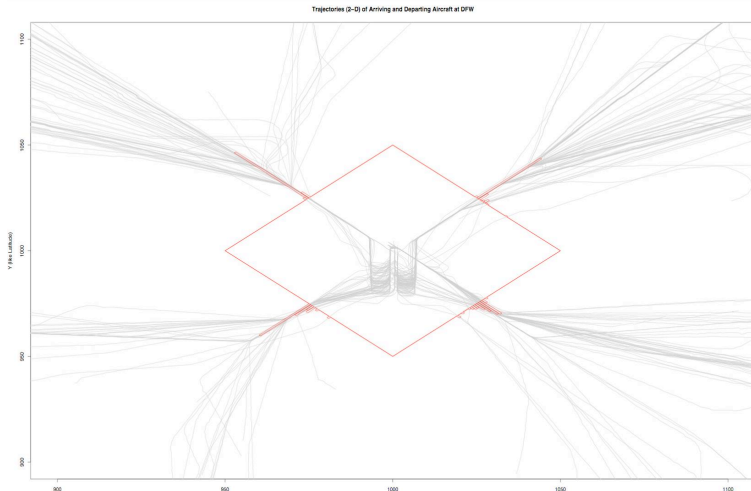
- ▶ Large Dimension: $1 \leq d \leq 1000$
- ▶ Huge Observations: $10^6 \leq n \leq 10^{10}$
- ▶ Need an **efficient** and **sufficient** multi-dimensional metric data-structure for non-parametric inference that is capable of:
 1. L_1 -consistent density estimation – adaptive histograms
 2. Extend Arithmetic over a dense class of Lipschitz \mathbb{M} -valued maps: $\{g : \mathbb{R}^d \rightarrow \mathbb{M}\}$ – functional estimation when $\mathbb{M} = \mathbb{R}$

└ Massive Metric Data Streams

└ Air Traffic Examples (Teng, Kuhn and S., *Jnl. Aerospace Comp., Inf. & Commun.*, [acc.] 2012)

Massive Metric Data Streams – Air Traffic Example

On a Sunny Day

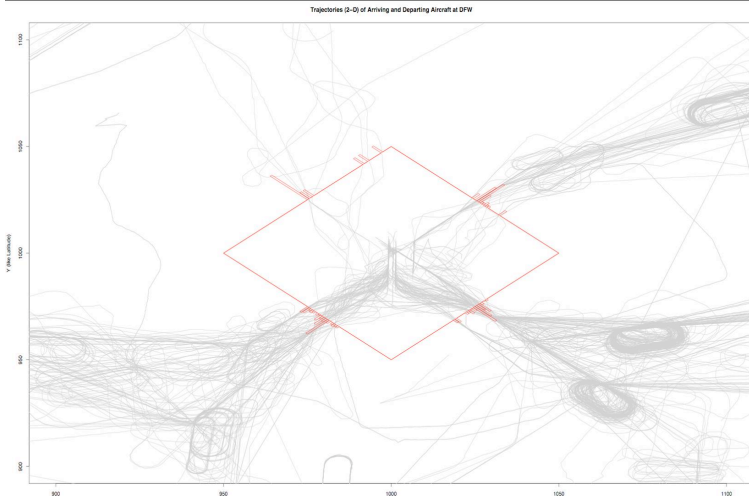


└ Massive Metric Data Streams

└ Air Traffic Examples (Teng, Kuhn and S., *Jnl. Aerospace Comp., Inf. & Commun.*, [acc.] 2012)

Massive Metric Data Streams – Air Traffic Example

On a Rainy Day

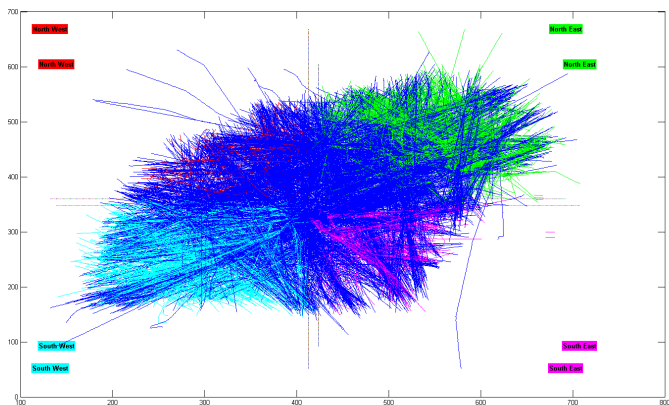


└ Massive Metric Data Streams

└ Air Traffic Examples (Teng, Kuhn and S., *Jnl. Aerospace Comp., Inf. & Commun.*, [acc.] 2012)

Massive Metric Data Streams – Air Traffic Example

We want to make sense of trajectories like these

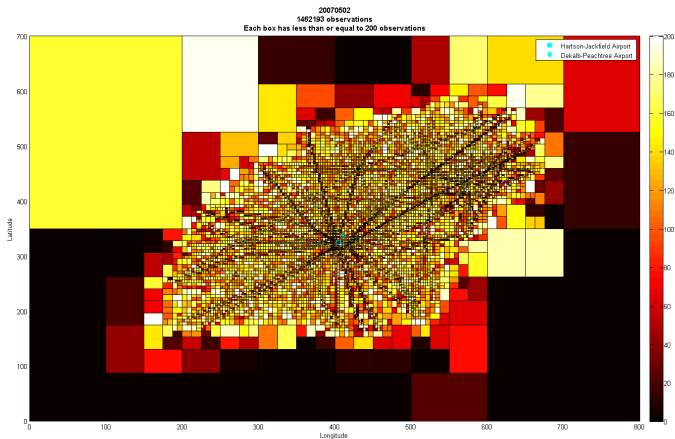


└ Massive Metric Data Streams

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Massive Metric Data Streams – Air Traffic Example

using a picture like this

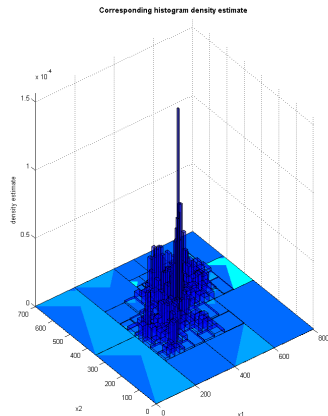
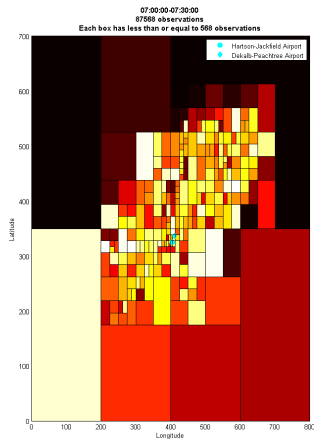


└ Massive Metric Data Streams

└ Air Traffic Examples (Teng, Kuhn and S., *Jnl. Aerospace Comp., Inf. & Commun.*, [acc.] 2012)

Massive Metric Data Streams – Air Traffic Example

A Histogram Estimate of Air-traffic between 0700 – 0730 hours

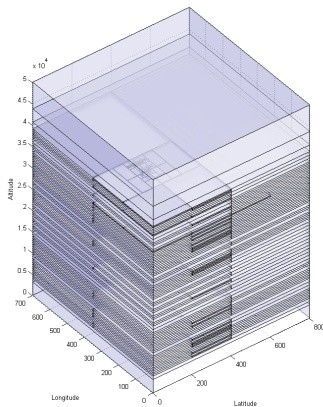
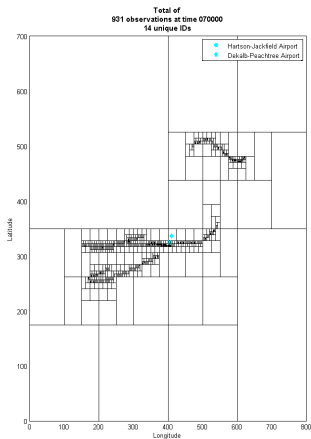


└ Massive Metric Data Streams

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Massive Metric Data Streams – Air Traffic Example

Add the pavings of 14 flight trajectories like this

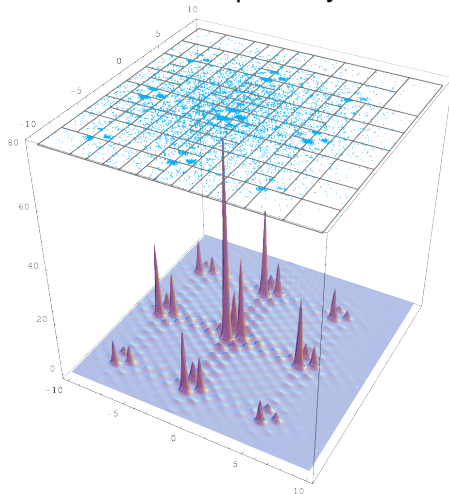


└ Massive Metric Data Streams

└ Synthetic Examples (Teng, Harlow, Lee and S., *ACM Trans. Mod. & Comp. Sim.*, [r. 2] 2012)

Massive Metric Data Streams – Synthetic Examples

Take millions of **realizations** of a possibly ‘challenging’ density

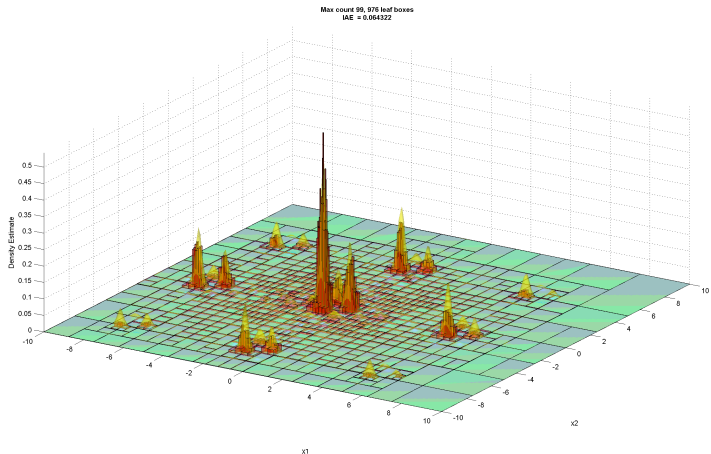


└ Massive Metric Data Streams

└ Synthetic Examples (Teng, Harlow, Lee and S., *ACM Trans. Mod. & Comp. Sim.*, [r. 2] 2012)

Massive Metric Data Streams – Synthetic Examples

and produce a consistent estimate of the density



Intervals and Boxes in \mathbb{R}^d

Intervals and *Boxes* as interval vectors:

$$\mathbf{x} = [\underline{x}_1, \bar{x}_1] \times [\underline{x}_2, \bar{x}_2] \times \dots \times [\underline{x}_d, \bar{x}_d], \quad \underline{x}_i \leq \bar{x}_i .$$

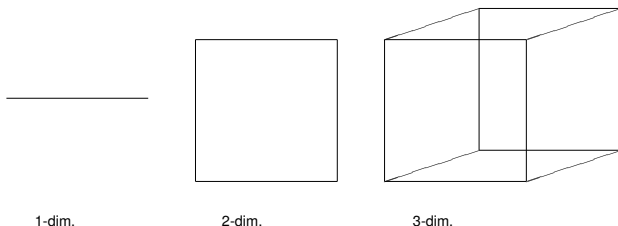


Figure : Boxes in 1D, 2D, and 3D.

Binary Tree Representation

These boxes can be represented by ordered binary trees, a.k.a.:

- *plane binary trees* of **enumerative combinatorics**
- *finite rooted binary (frb-trees)* of **geometric group theory**

An operation of bisection on a box is equivalent to performing the operation on its corresponding node in the tree:

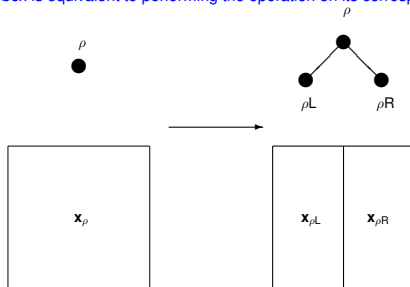
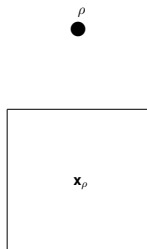


Figure : Bisecting a box or its equivalent node.

Regular Pavings (RPs)

- ▶ A sequence of bisections of boxes;
- ▶ Start from the root box;
- ▶ Along the first widest dimension.

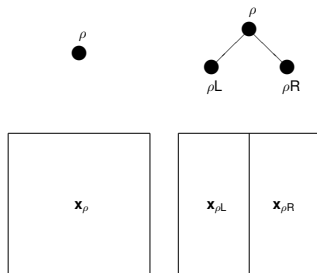
A sequence of bisections on root box \mathbf{x} to get a 4-leaved RP.



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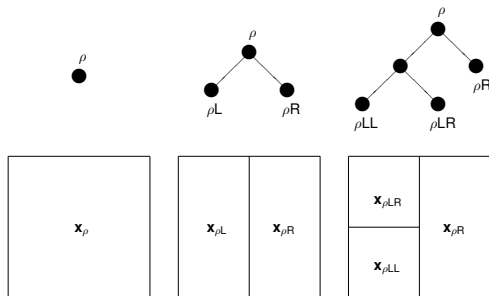
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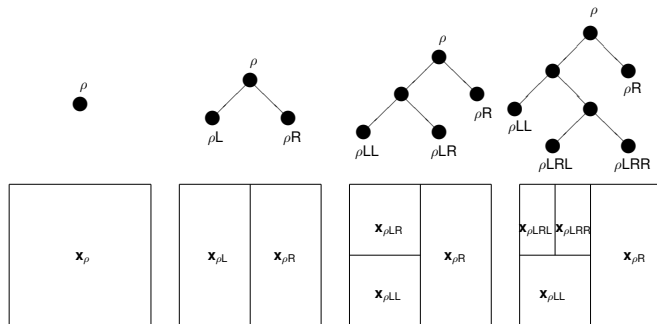
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A sequence of bisections on root box \mathbf{x} to get a 4-leaved RP.

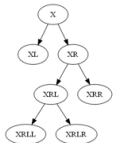


State Space of Regular Pavings

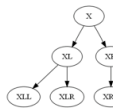
Leaf-depth encoded RPs



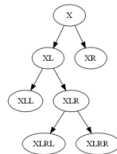
(3, 3, 2, 1)



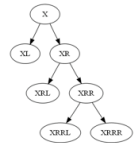
(1, 3, 3, 2)



(2, 2, 2, 2)



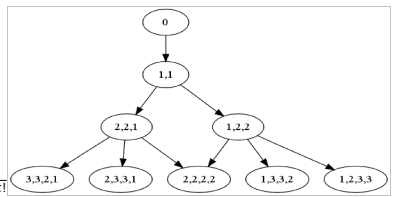
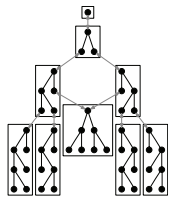
(2, 3, 3, 1)



(1, 2, 3, 3)

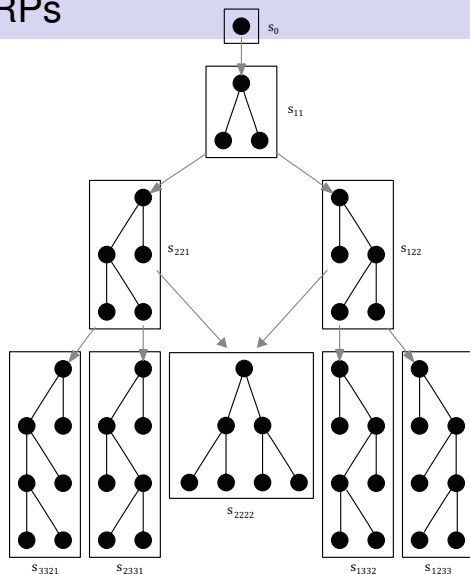
C_k RPs with k splits

- $C_0 = 1$
- $C_1 = 1$
- $C_2 = 2$
- $C_3 = 5$
- $C_4 = 14$
- $C_5 = 42$
- $C_k = \frac{(2k)!}{(k+1)!k!}$



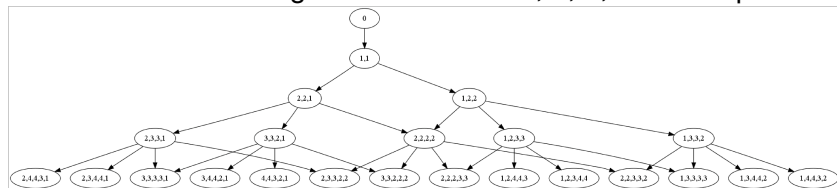
The Space of All Possible RPs

- ▶ Let \mathcal{S}_i be the set of all RPs of \mathbf{x} made of i splits and
- ▶ Let $\mathcal{S}_{i:j}$ be the set of RPs with k splits where $k \in \{i, i+1, \dots, j\}$
- ▶ The space of all RPs is $\mathcal{S}_{0:\infty} := \lim_{j \rightarrow \infty} \mathcal{S}_{0:j}$
- ▶ RPs are closed under pair-wise union (or overlay) operations (Thompson's Group)
- ▶ can get as m_∞ -close as desired to any subset of \mathbf{x}



State Transition Diagram of Regular Pavings

State Transition Diagram of RPs with 0, 1, 2, 3 and 4 splits.



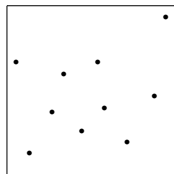
1. The above state space is denoted by $\mathbb{S}_{0:4}$
2. Number of RPs with k splits is the Catalan number C_k
3. There is more than one way to reach a RP by k splits
4. Randomized algorithms here are Markov chains on $\mathbb{S}_{0:\infty}$

Statistical Regular Pavings (SRPs)

- ▶ Extended from the RP;
- ▶ Caches recursively computable statistics at each box or node as data falls through;
- ▶ These statistics include:
 - ▶ the sample count;
 - ▶ the sample mean vector;
 - ▶ the sample variance-covariance matrix;
 - ▶ and the volume of the box.

Caching the sample count in each node (or box).

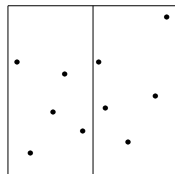
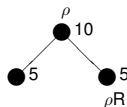
ρ
● 10



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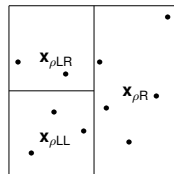
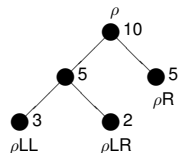
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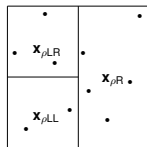
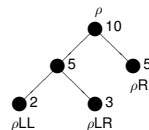
SRPs as Adaptive Histograms

SRP estimate of f from random vectors $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} f$ is

$$f_{n,\dot{s}}(x) = \frac{1}{n} \sum_{i=1}^n \frac{\mathbb{1}(x_i \in \mathbf{x}(x))}{\text{vol}(\mathbf{x}(x))},$$

$\mathbf{x}(x) \in \ell(\dot{s})$ is the leaf box containing x with volume $\text{vol}(\mathbf{x}(x))$

Figure : A SRP as a histogram estimate.



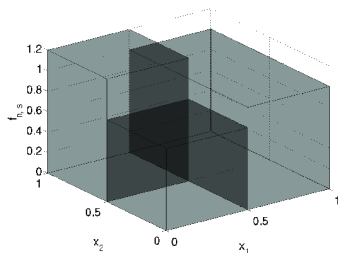
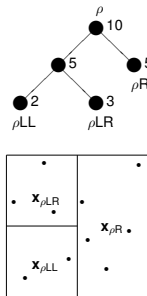
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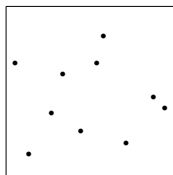


A Prioritized Queue based Algorithm

Algorithm `SplitMostCounts`

As data arrives, order the leaf boxes of the SRP so that the leaf box with **the most number of points** will be chosen for the next bisection.

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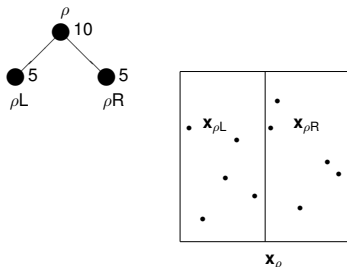
\mathbf{x}_ρ

A Prioritized Queue based Algorithm

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Split the root box.

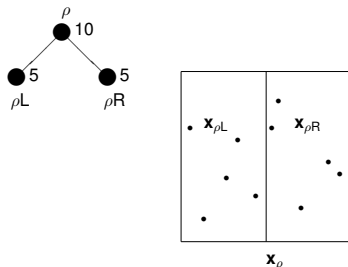


A Prioritized Queue based Algorithm

Algorithm `SplitMostCounts`

As data arrives, order the leaf boxes of the SRP so that the leaf box with **the most number of points** will be chosen for the next bisection.

Two or more boxes with the most number of points?

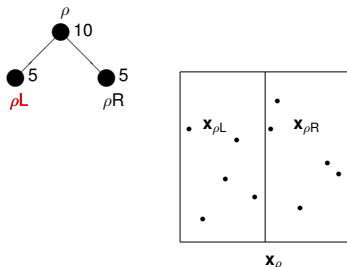


A Prioritized Queue based Algorithm

Algorithm `SplitMostCounts`

As data arrives, order the leaf boxes of the SRP so that the leaf box with **the most number of points** will be chosen for the next bisection.

Break such ties by randomising the next bisection.

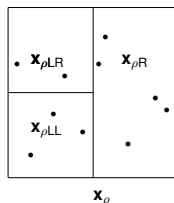
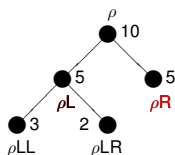


A Prioritized Queue based Algorithm

Algorithm `SplitMostCounts`

As data arrives, order the leaf boxes of the SRP so that the leaf box with **the most number of points** will be chosen for the next bisection.

Bisect until each box has $\leq \bar{k}_n$ points (let $\bar{k}_n = 3$ here).

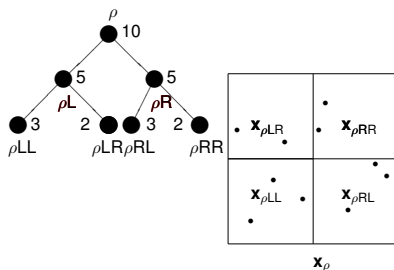


A Prioritized Queue based Algorithm

Algorithm `SplitMostCounts`

As data arrives, order the leaf boxes of the SRP so that the leaf box with **the most number of points** will be chosen for the next bisection.

Final state



The SplitMostCounts Algorithm

Input: (i) data: $\mathbf{x}_1, \dots, \mathbf{x}_n \subseteq \mathbb{R}^d$; (ii) root box: \mathbf{x}_ρ // optional;
 (iii) padding to handle pulsed data: $\psi \geq 0$ // optional;
 (iv) S.E.B. max: \bar{k}_n ; (v) maximum partition size: \bar{m}_n .
Output: histogram estimate $f_{n,s}$.

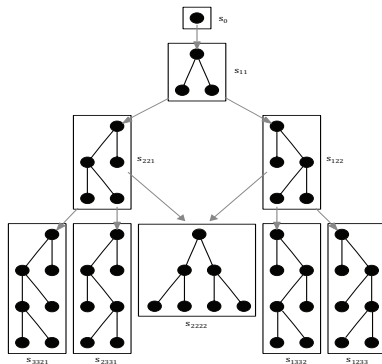
```

initialize  $i \leftarrow 1$ ;  $\mathbf{s} \leftarrow \mathbf{x}_\rho + \psi$ ;
repeat until
   $\#\mathbf{x}_{\rho v} \leq \bar{k}_n$  for each  $\mathbf{x}_{\rho v} \in \ell(\mathbf{s})$  and  $i \leq \bar{m}_n$  //
 $\ell(\mathbf{s}) = \{\text{leaf boxes}\}$ 
   $\mathbf{x}_{\rho v} \leftarrow \text{Uniform}(\hat{\ell}(\mathbf{s}))$  // randomized PQ on leaf boxes
   $\mathbf{s} \leftarrow \text{bisect}(\mathbf{s}, \mathbf{x}_{\rho v})$  // bisect leaf box  $\mathbf{x}_{\rho v}$  of  $\mathbf{s}$ 
  recursively update counts in  $\mathbf{s}$ ;
   $i \leftarrow i + 1$ ;
return  $f_{n,s}$ .
  
```

- └ Adaptive Histograms
- └ S.E.B. Priority Queue

Transition Diagram of Randomized PQ Markov chain

Let \mathcal{S}_i be the set of all RPs of \mathbf{x}_ρ made of i splits and for $i, j \in \mathbb{N}$ with $i \leq j$, let $\mathcal{S}_{i:j}$ be the set of RPs with k splits, $i \leq k \leq j$.



All possible RP partitions in $\mathcal{S}_{0:4}$.

Proposition: L_1 -Consistency of Histogram Estimates from SplitMostCounts

Let X_1, X_2, \dots be independent and identical random vectors in \mathbb{R}^d whose common distribution μ has a non-atomic density f , i.e., $f \ll \lambda^d$. Let $\{S_n(i)\}_{i=0}^j$ on $\mathbb{S}_{0:\infty}$ be the Markov chain formed using SplitMostCounts with terminal state \dot{s} and histogram estimate $f_{n,\dot{s}}$ over the collection of partitions \mathcal{L}_n .

As $n \rightarrow \infty$, if $\bar{k}_n \rightarrow \infty$, $n^{-1}\bar{k}_n \rightarrow 0$, $\bar{m}_n \geq n/\bar{k}_n$, and $\bar{m}_n/n \rightarrow 0$ then the density estimate $f_{n,\dot{s}}$ is strongly consistent in L_1 , i.e.

$$\int |f(x) - f_{n,\dot{s}}(x)| dx \rightarrow 0 \text{ with probability 1.}$$

Proof Sketch

We will assume that $\bar{k}_n \rightarrow \infty$, $n^{-1}\bar{k}_n \rightarrow 0$, $\bar{m}_n \geq n/\bar{k}_n$, and $\bar{m}_n/n \rightarrow 0$, as $n \rightarrow \infty$, and show that the three conditions:

- (a) $n^{-1}m(\mathcal{L}_n) \rightarrow 0$,
- (b) $n^{-1} \log \Delta_n^*(\mathcal{L}_n) \rightarrow 0$, and
- (c) $\mu(\mathbf{x} : \text{diam}(\mathbf{x}(x)) > \gamma) \rightarrow 0$ with probability 1 for every $\gamma > 0$,

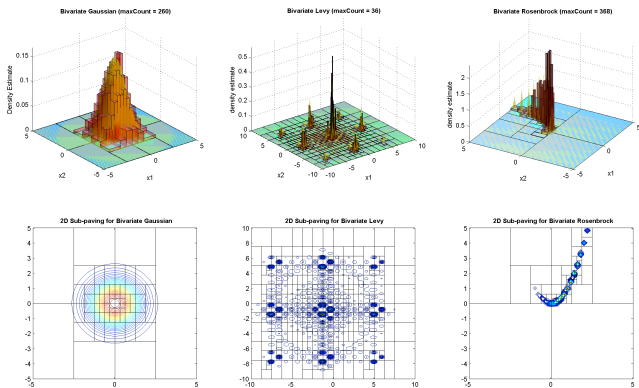
are satisfied. Then by Theorem 1 of Lugosi and Nobel, 1996 our density estimate $f_{n,\hat{s}}$ is strongly consistent in L_1 .

These conditions mean:

- (a) sub-linear growth of the number of leaf boxes
- (b) sub-exponential growth of a combinatorial complexity measure of the growth of the partition
- (c) shrinking leaf boxes in the partition

Some Examples

Figure : Histogram density estimates their corresponding pavings for the bivariate Gaussian, Levy and Rosenbrock densities.



Choice of k_n

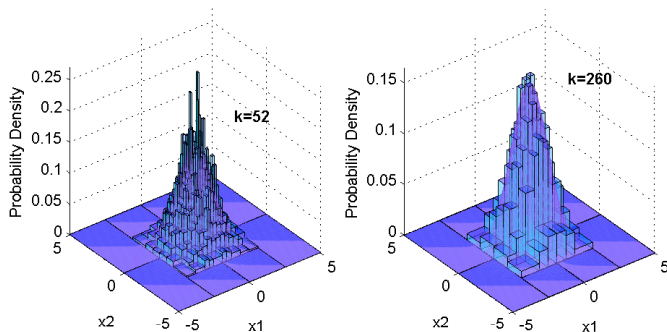


Figure : Two histogram density estimates for the standard bivariate gaussian density with different choices of k_n . The histogram is under-smoothed when k_n is relatively smaller than n and over-smoothed when k_n is relatively larger.

Adding and Averaging SRPs

Do a minimal union (or overlay) operation of $s^{(1)}$ and $s^{(2)}$ with root nodes $\rho^{(1)}$ and $\rho^{(2)}$, and add the value $h(\rho v)$ for each leaf box ρv :

$$\begin{array}{|c|c|} \hline \rho^{(1)} & \\ \hline h(\rho^{(1)}LR) & \\ \hline h(\rho^{(1)}LL) & h(\rho^{(1)}R) \\ \hline \end{array} + \begin{array}{|c|c|} \hline \rho^{(2)} & \\ \hline & h(\rho^{(2)}RR) \\ \hline h(\rho^{(2)}L) & \\ \hline & h(\rho^{(2)}RL) \\ \hline \end{array} =$$

Adding and Averaging SRPs

Do a minimal union (or overlay) operation of $s^{(1)}$ and $s^{(2)}$ with root nodes $\rho^{(1)}$ and $\rho^{(2)}$, and add the value $h(\rho v)$ for each leaf box ρv :

$$\begin{array}{|c|c|} \hline \rho^{(1)} & \\ \hline h(\rho^{(1)}LR) & \\ \hline h(\rho^{(1)}LL) & h(\rho^{(1)}R) \\ \hline \end{array}
 +
 \begin{array}{|c|c|} \hline \rho^{(2)} & \\ \hline & h(\rho^{(2)}RR) \\ \hline h(\rho^{(2)}L) & \\ \hline & h(\rho^{(2)}RL) \\ \hline \end{array}
 =
 \begin{array}{|c|c|} \hline \rho^{(1)+(2)} & \\ \hline h(\rho^{(1)}LR) & h(\rho^{(1)}R) \\ +h(\rho^{(2)}L) & +h(\rho^{(2)}RR) \\ \hline h(\rho^{(1)}LL) & h(\rho^{(1)}R) \\ +h(\rho^{(2)}L) & +h(\rho^{(2)}RL) \\ \hline \end{array}$$

Adding and Averaging SRPs

Adding m SRP histogram density estimates

$$\begin{aligned}\sum_{i=1}^m f_{n,s^{(i)}} &= f_{n,s^{(1)}} + f_{n,s^{(2)}} + f_{n,s^{(3)}} + \dots + f_{n,s^{(m)}} \\ &= \left(\left(\left(f_{n,s^{(1)}} + f_{n,s^{(2)}} \right) + f_{n,s^{(3)}} \right) + \dots + f_{n,s^{(m)}} \right) .\end{aligned}$$

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Averaging m SRP histogram density estimates recursively yields the sample mean SRP histogram

$$\bar{f}_{n,m} = \frac{1}{m} \sum_{i=1}^m f_{n,s^{(i)}} .$$

An Example

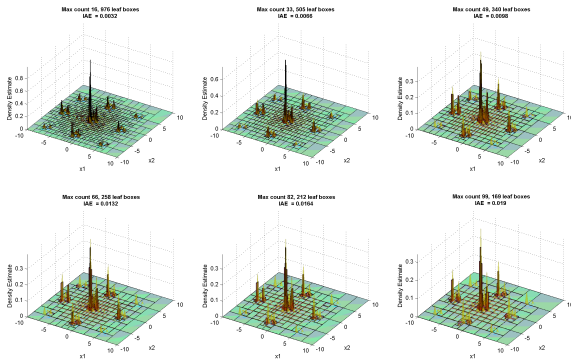


Figure : Histogram density estimates of the bivariate Levy using different values of \bar{k}_n .

An Example

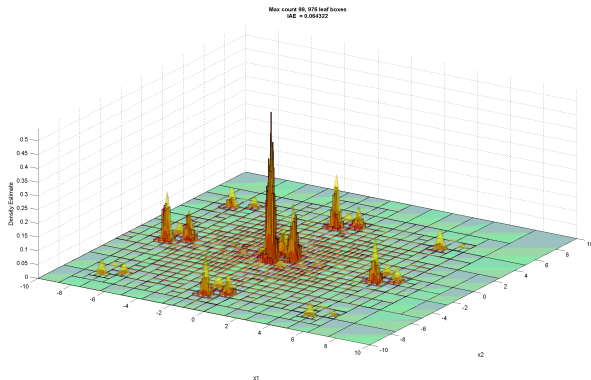


Figure : The averaged histogram density estimate.

Posterior Distribution over Histograms in $\mathbb{S}_{0:\infty}$

- ▶ Let \hat{f}_s be a histogram with partition $\ell(s)$ given by the leaves of RP s with k splits and $k + 1$ leaves in \mathbb{S}_k

Posterior Distribution over Histograms in $\mathbb{S}_{0:\infty}$

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- ▶ Then for this partition, the most likely histogram estimate is

$$\hat{f}_s(x; \text{data}) = \frac{1}{n} \hat{f}_s(x; X_{1:n}) = \sum_{i=1}^n \frac{\mathbf{1}(x_i \in \mathbf{x}(x))}{\text{vol}(\mathbf{x}(x))}$$

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- ▶ Let the prior probability be $P(s) \propto \frac{1}{C_k^2}$, $s \in \mathbb{S}_{0:\infty}$
- ▶ Then the posterior density of histogram \hat{f}_s with k splits is

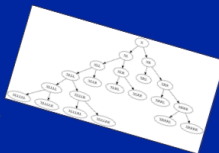
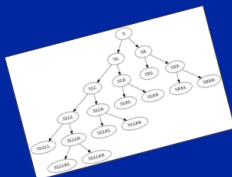
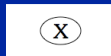
$$P(\hat{f}_s | X_{1:n}) \propto P(X_{1:n} | s) P(s) = \prod_{\mathbf{x}_{\rho\nu} \in \ell(s)} \left(\frac{\#\mathbf{x}_{\rho\nu}}{n \text{vol}(\mathbf{x}_{\rho\nu})} \right)^{n_{\mathbf{x}_{\rho\nu}}} \frac{1}{C_k^2}$$

Metropolis-Hastings Algorithm

- ▶ Use a proposal density $q(s^{prime}|s^{(i)})$ which depends on current state $s^{(i)}$, to generate a new proposed state s'
- ▶ We propose uniformly at random to split a leaf or merge a cherry of current SRP state $s^{(i)}$
- ▶ **Repeat**
 - ▶ **Draw** $u \sim U(0, 1)$
 - ▶ **If** $u < \frac{P(\hat{f}_{s'}|X_{1:n})}{P(\hat{f}_{s^{(i)}}|X_{1:n})} \frac{q(s^{(i)}|s')}{q(s^{prime}|s^{(i)})}$ **then** $s^{(i+1)} \leftarrow s'$
 - ▶ **else** $s^{(i+1)} \leftarrow s^{(i)}$
- ▶ With a “long enough” burn-in time, this Markov chain will be at the desired stationary distribution $P(\hat{f}_s|X_{1:n})$ over $\mathbb{S}_{0:\infty}$

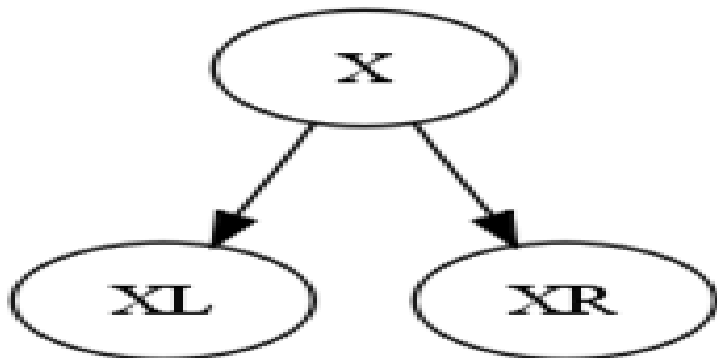
Metropolis-Hastings Algorithm

- Start from some initial state m^0
- Burn-in: run until initial state is 'forgotten'
- States after burn-in are sample histograms

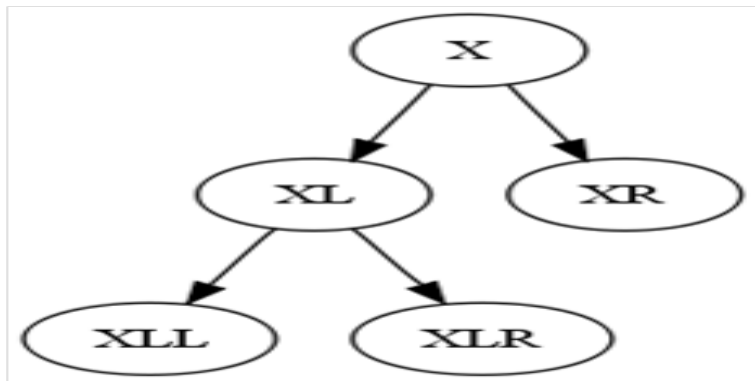


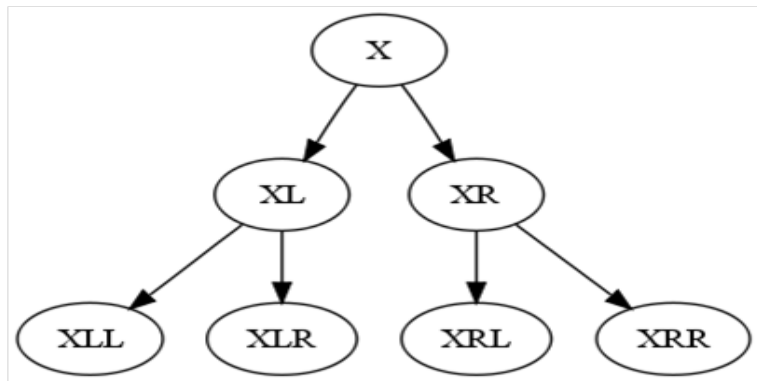
etc...

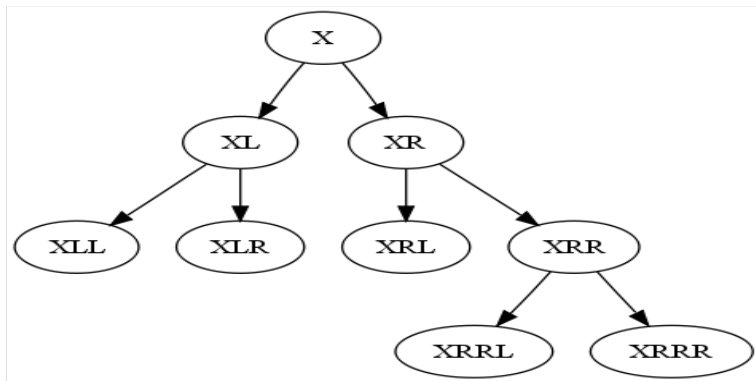
Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$

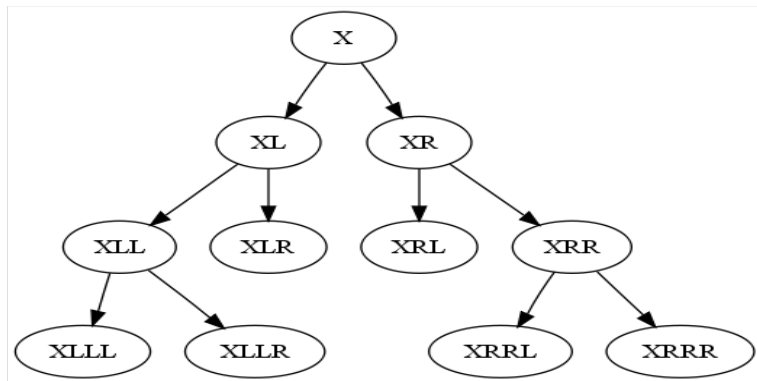


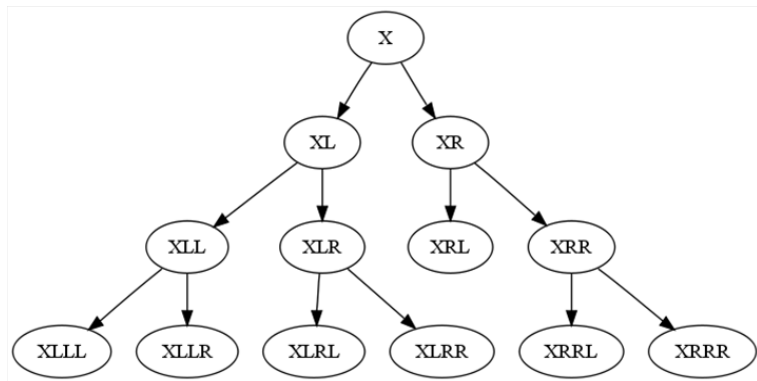
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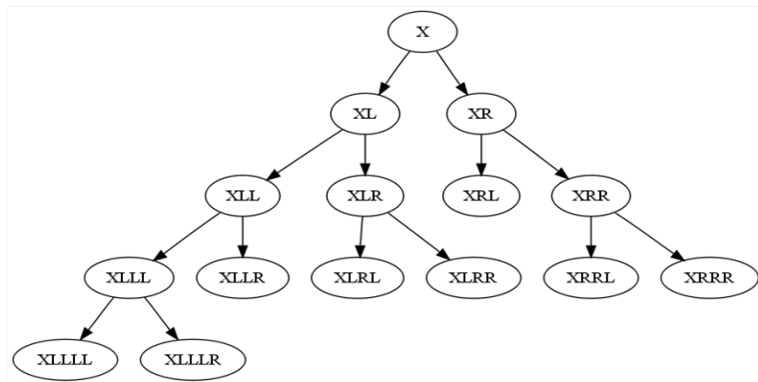


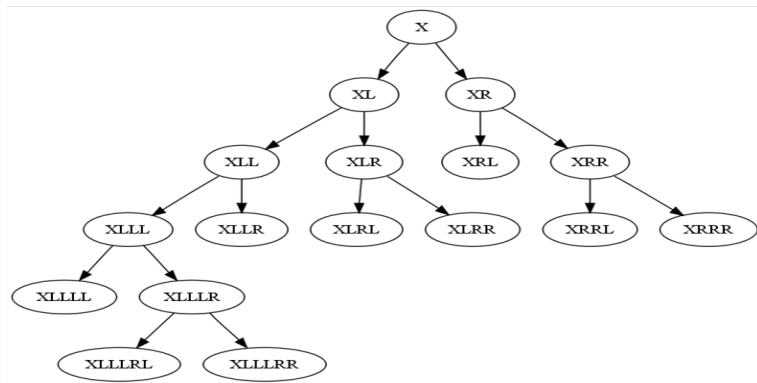
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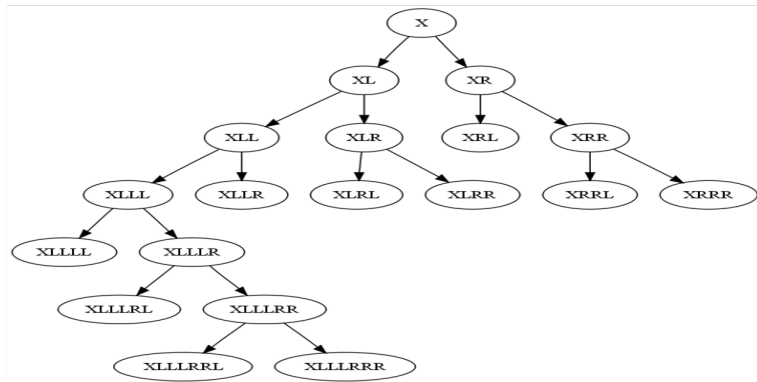
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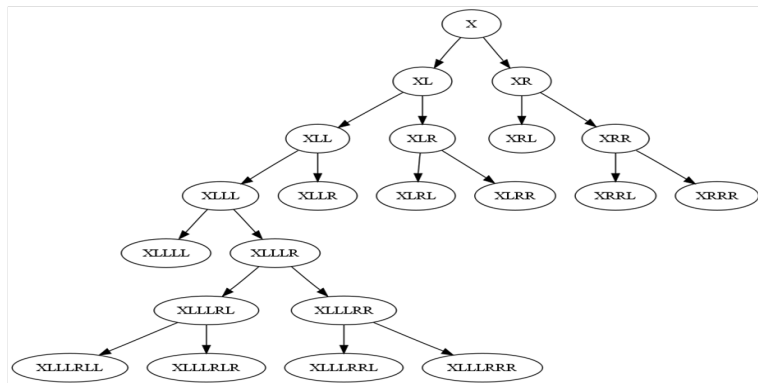
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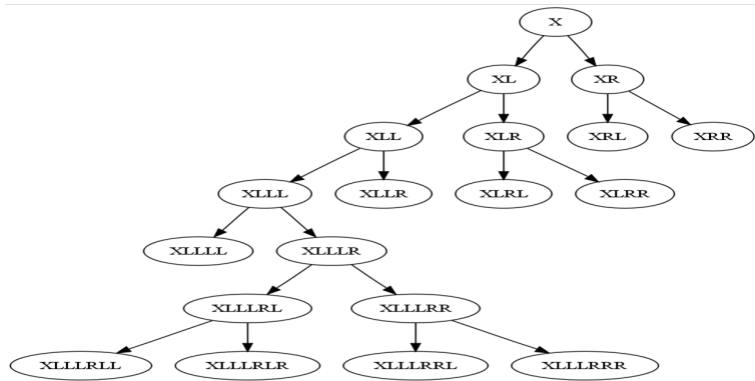
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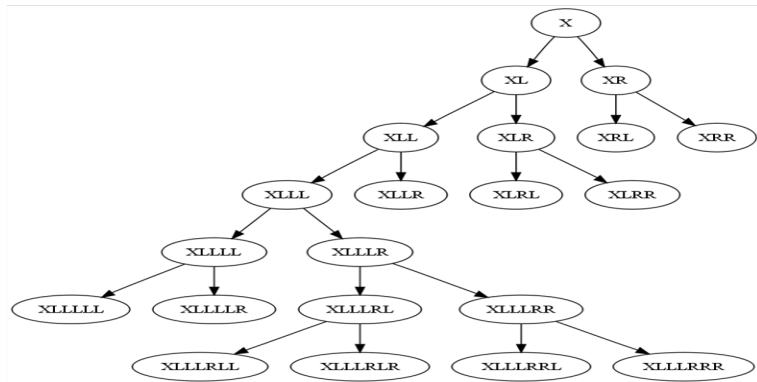
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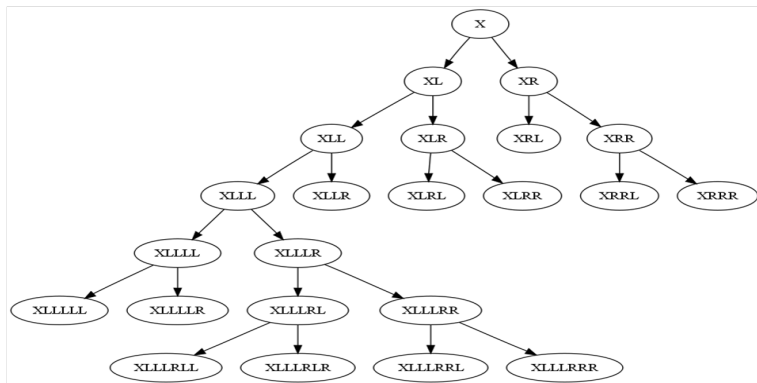
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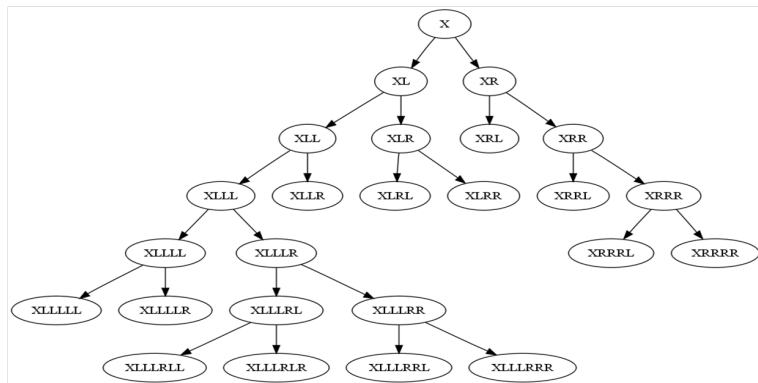


Monte Carlo Markov Chain over Histograms in $\mathcal{S}_{0:\infty}$ 

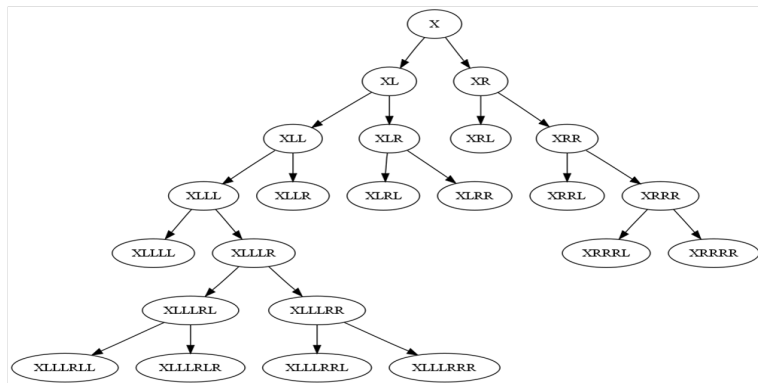
Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



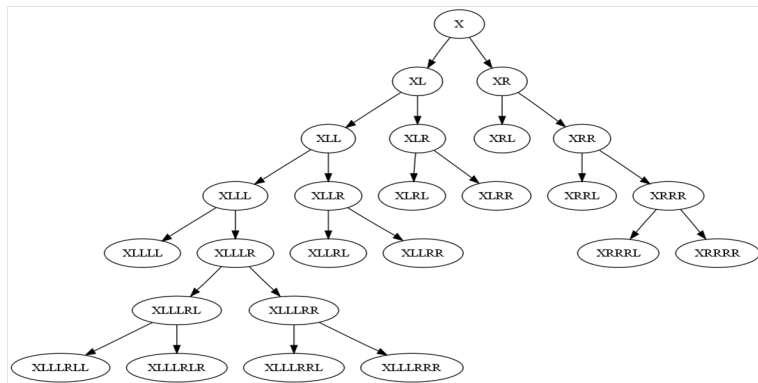
Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



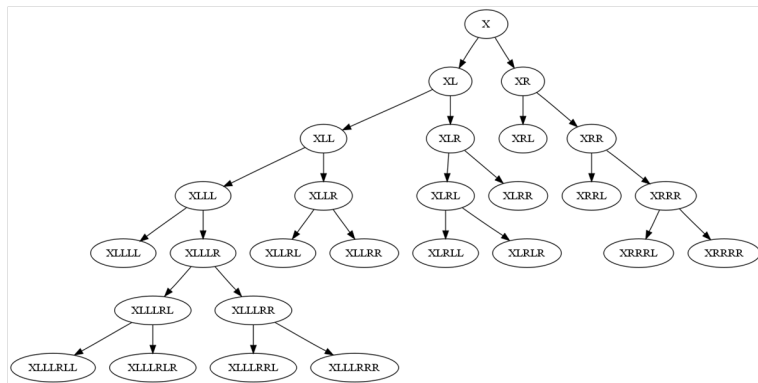
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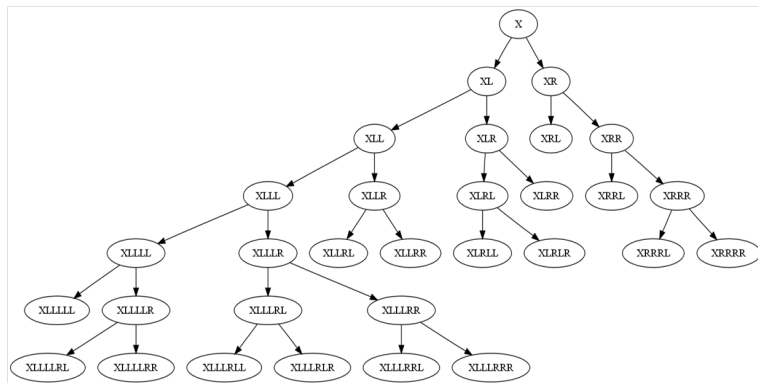
Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



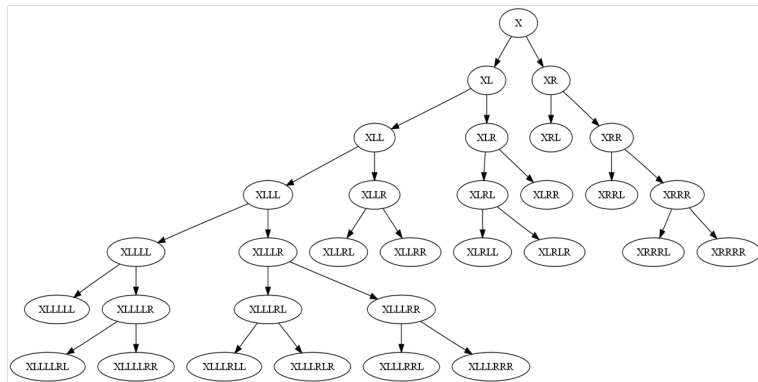
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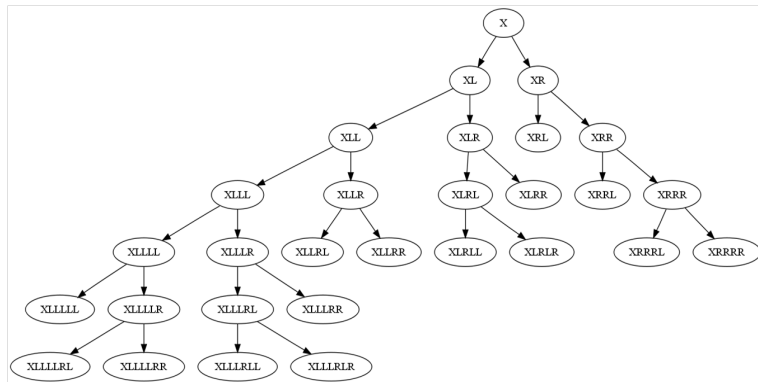
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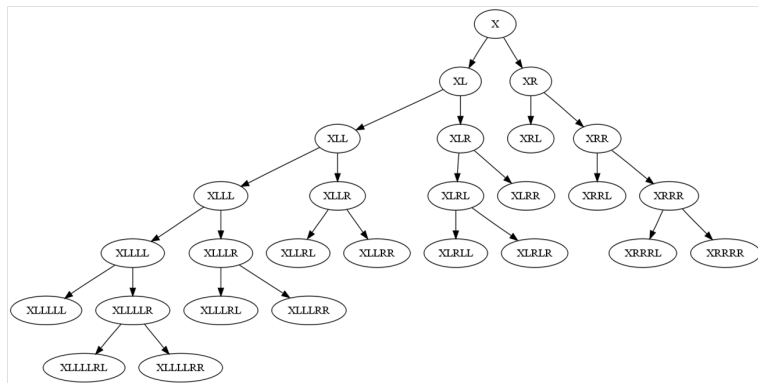
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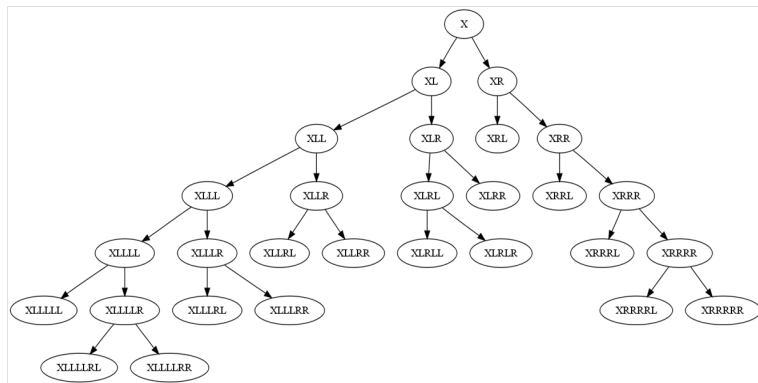
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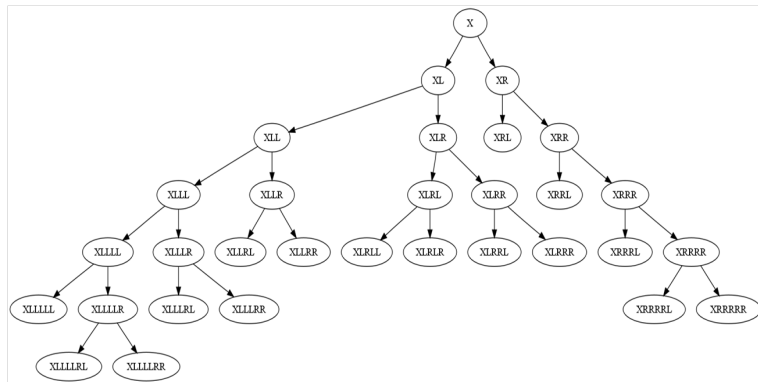
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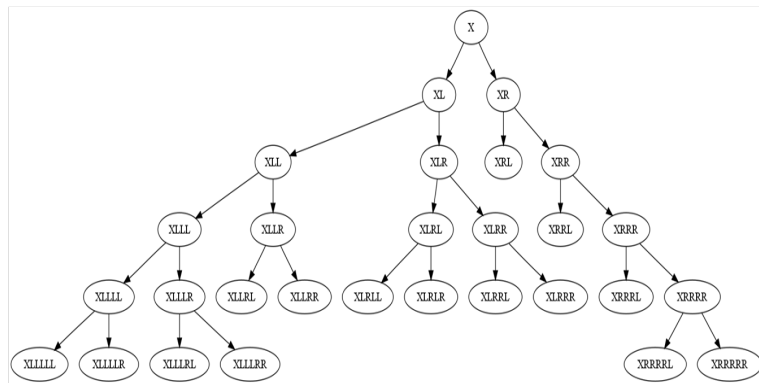


Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$

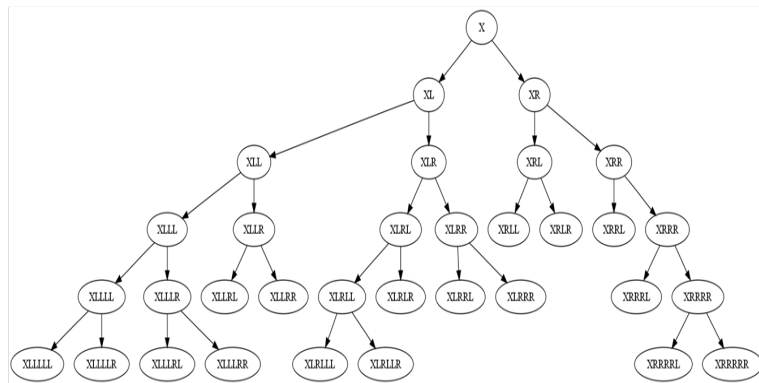


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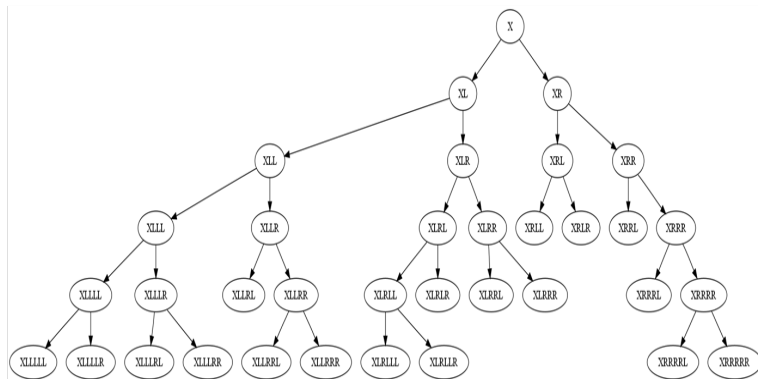
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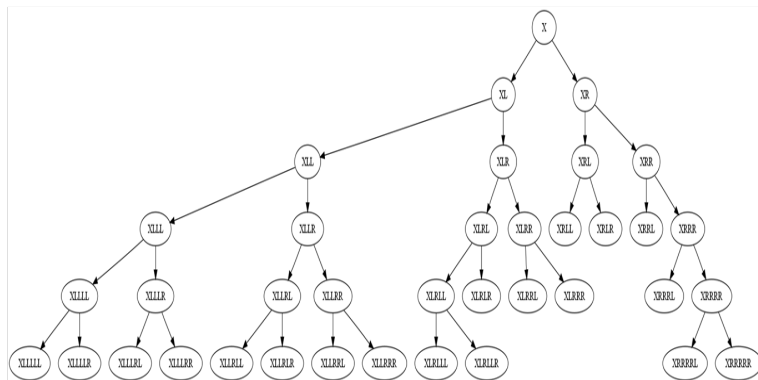
└ Posterior Expectation over Histograms in $\mathbb{S}_{0:\infty}$

Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



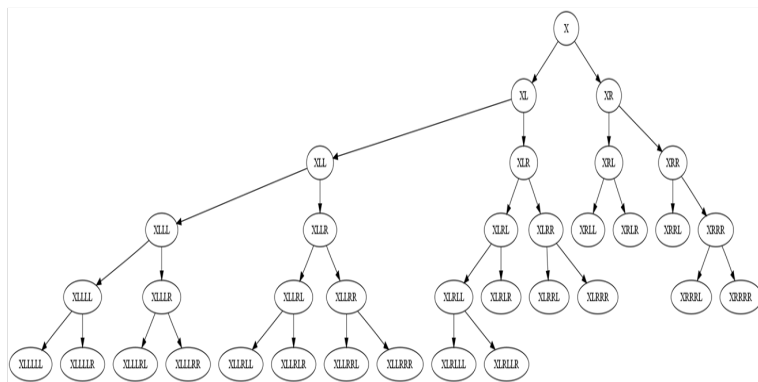
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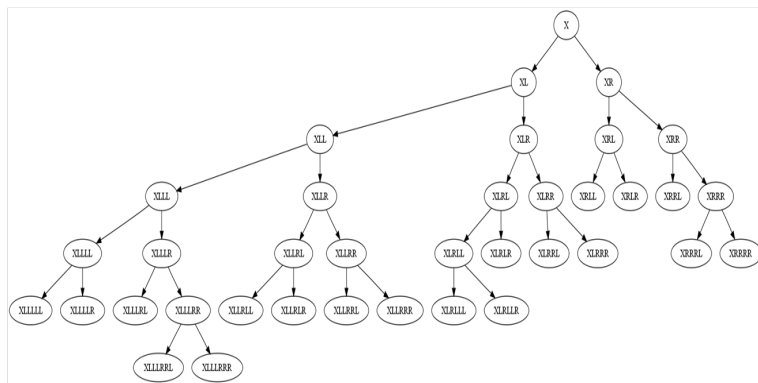
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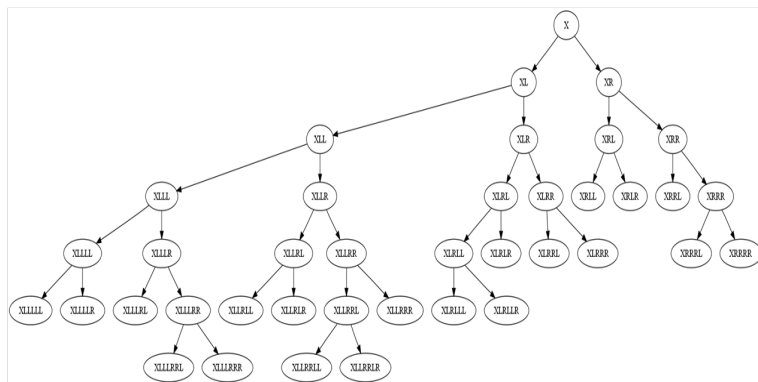
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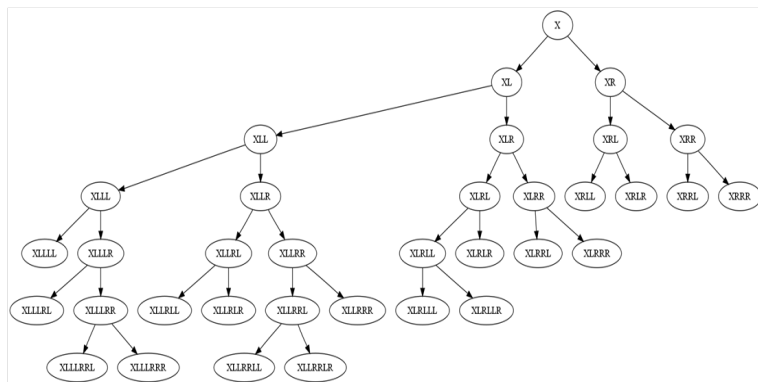


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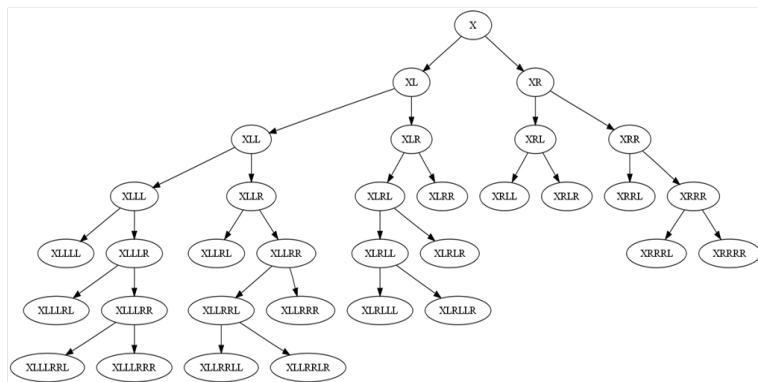
Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$

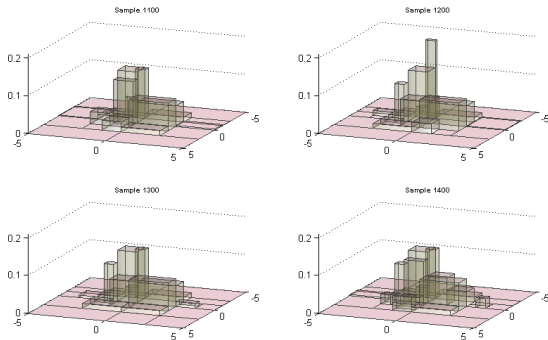


Monte Carlo Markov Chain over Histograms in $\mathbb{S}_{0:\infty}$



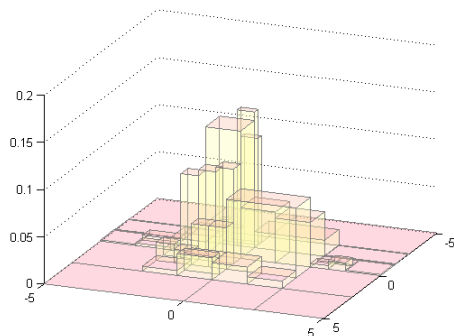
└ Examples - good, bad and ugly

Histogram Estimates - Standard Bivariate Gaussian



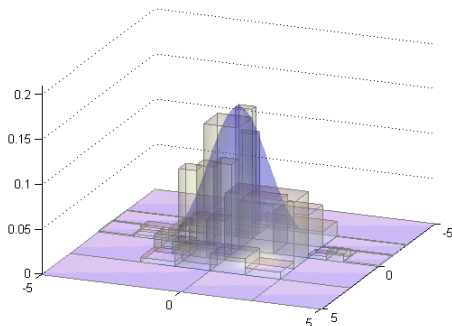
Four sample histograms

Histogram Estimates - Standard Bivariate Gaussian



Average of the four sampled histograms

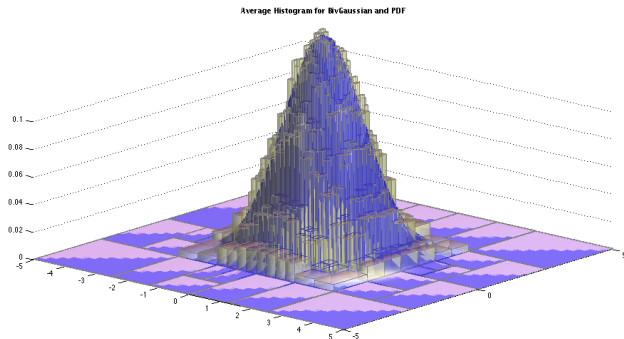
Histogram Estimates - Standard Bivariate Gaussian



Average of the four sampled histograms with Gaussian PDF

└ Examples - good, bad and ugly

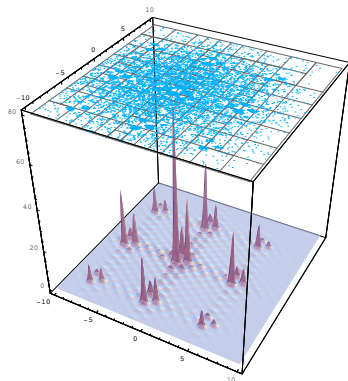
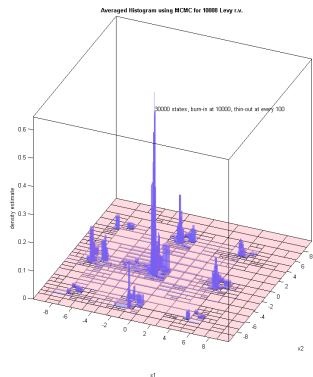
Histogram Estimates - Standard Bivariate Gaussian



A much better estimate

└ Examples - good, bad and ugly

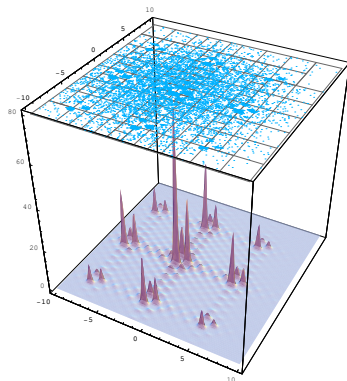
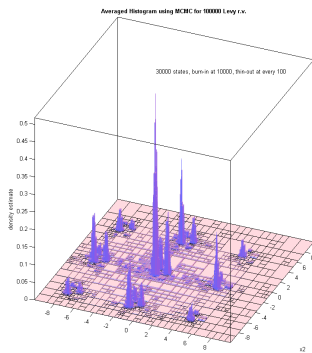
Histogram Estimates - Bivariate Levy Density



Data points = 10000, Number of states = 30000, Burn-in = 10000,
Thin-out = 100, Averaged over 201 states, Time taken = 14.16s

└ Examples - good, bad and ugly

Histogram Estimates - Bivariate Levy Density



Data points = 100000, Number of states = 30000, Burn-in = 10000,
Thin-out = 100, Averaged over 201 states, Time taken = 50.59s

Simulations for MCMC and `SplitMostCounts` PQ

MIAE (std. err.) for n samples from uniform density in various dimensions (CPU Times $< O(1\text{minute})$).

n	1D	2D	10D	100D	1000D
10^2	0.1112 (0.0707)	0.1425 (0.0882)	0.1170 (0.0723)	0.0958 (0.0605)	0.1111 (0.0524)
10^3	0.0366 (0.0192)	0.0363 (0.0219)	0.0442 (0.0275)	0.0413 (0.0196)	0.0305 (0.0195)
10^4	0.0164 (0.0095)	0.0124 (0.0073)	0.0115 (0.0070)	0.0111 (0.0083)	0.0089 (0.0065)
10^5	0.0041 (0.0020)	0.0040 (0.0026)	0.0041 (0.0028)	0.0050 (0.0030)	0.0043 (0.0025)
10^6	0.0011 (0.0005)	0.0016 (0.0007)	0.0010 (0.0006)	0.0012 (0.0001)	0.0010 (0.0004)
10^7	0.0004 (0.0003)	0.0003 (0.0002)	0.0003 (0.0002)	0.0002 (0.0001)	-
10^8	0.0001 (0.0009)	0.0002 (0.0002)	0.0001 (0.0001)	-	-

└ Examples - good, bad and ugly

Simulations for MCMC and `SplitMostCounts` PQ

MIAE (std. err.) for n samples from approximated 1D-, 2D- and 10D-Gaussian densities, and 2D- and 10D-Rosenbrock densities (L_1 -minimal Simple function approximation in \mathbb{S}_λ).

λ	n	Standard Gaussian densities			Rosenbrock densities	
		1D	2D	10D	2D	10D
10^2	10^2	0.2665 (0.0415)	0.4856 (0.0491)	0.1192 (0.0662)	0.5089 (0.0924)	0.0323 (0.0511)
	10^3	0.1390 (0.0192)	0.2558 (0.0127)	0.0543 (0.0172)	0.1712 (0.0224)	0.0095 (0.0191)
	10^4	0.0620 (0.0047)	0.0992 (0.0067)	0.0382 (0.0036)	0.0498 (0.0081)	0.0025 (0.0050)
	10^5	0.0262 (0.0016)	0.0279 (0.0019)	0.0259 (0.0017)	0.0143 (0.0025)	0.0009 (0.0015)
	10^6	0.0099 (0.0008)	0.0086 (0.0006)	0.0073 (0.0009)	0.0045 (0.0005)	0.0004 (0.0005)
	10^7	0.0026 (0.0002)	0.0027 (0.0003)	0.0025 (0.0004)	0.0017 (0.0010)	0.0001 (0.0003)
	10^3	10^2	0.2946 (0.0678)	0.6046 (0.1299)	0.1702 (0.0907)	1.0027 (0.0437)
10^3		0.1418 (0.0226)	0.2973 (0.0174)	0.0739 (0.0183)	0.4747 (0.0191)	0.0039 (0.0075)
10^4		0.0648 (0.0052)	0.1586 (0.0067)	0.0555 (0.0045)	0.2139 (0.0054)	0.0013 (0.0028)
10^5		0.0292 (0.0014)	0.0768 (0.0016)	0.0295 (0.0020)	0.0789 (0.0023)	0.0004 (0.0006)
10^6		0.0136 (0.0006)	0.0297 (0.0006)	0.0108 (0.0005)	0.0267 (0.0058)	0.0001 (0.0002)
10^7		0.0061 (0.0002)	0.0091 (0.0003)	0.0045 (0.0003)	0.0082 (0.0011)	0.0001 (0.0002)
10^4		10^2	0.2864 (0.0487)	0.5508 (0.0590)	0.5210 (0.0799)	1.1391 (0.0545)
	10^3	0.1380 (0.0152)	0.3301 (0.0120)	0.2719 (0.0251)	0.6018 (0.0139)	0.0791 (0.0223)
	10^4	0.0664 (0.0062)	0.1736 (0.0038)	0.1157 (0.0047)	0.3163 (0.0047)	0.0391 (0.0041)
	10^5	0.0293 (0.0017)	0.0957 (0.0014)	0.0870 (0.0014)	0.1691 (0.0053)	0.0209 (0.0021)
	10^6	0.0138 (0.0005)	0.0495 (0.0005)	0.0788 (0.0009)	0.0882 (0.0048)	0.0123 (0.0012)
	10^7	0.0063 (0.0001)	0.0244 (0.0008)	0.0563 (0.0018)	0.0479 (0.0057)	0.0096 (0.0017)

Minimum Distance Estimation (MDE)

- ▶ Let θ be the current number of splits in `SplitMostCounts`.
- ▶ Let $f_{n,\theta}$ be the histogram estimate with corresponding SRP $\mathbf{s} \in \mathbb{S}_\theta$, $\int f_{n,\theta} = 1$.
- ▶ Denote Θ as the set of the number of splits such that $\Theta := \{0, \dots, \bar{m}_n - 1\}$ where $\bar{m}_n - 1$ is the maximum number of splits allowed.

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The goal is to select the optimal estimate amongst the $|\Theta|$ candidates, $f_{n,\theta}, \theta \in \Theta$ by using a hold-out method proposed by Devroye and Lugosi, 2004 for minimum distance estimation (MDE).

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Scheffé set

For a pair (θ, θ') , $\theta, \theta' \in \Theta$, $\theta \neq \theta'$, the Scheffé set is

$$A_{\theta, \theta'} := A(f_{n-\varphi n, \theta}, f_{n-\varphi n, \theta'}) = \{x : f_{n-\varphi n, \theta}(x) > f_{n-\varphi n, \theta'}(x)\} .$$

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Yatracos class

The class of all sets of the form $A_{\theta, \theta'}$:

$$\mathcal{A}_{\Theta} := \left\{ \{x : f_{n-\varphi n, \theta}(x) > f_{n-\varphi n, \theta'}(x)\} : \theta, \theta' \in \Theta, \theta \neq \theta' \right\} .$$

Minimum Distance Estimation (MDE)

Minimum distance estimate

The minimum distance estimate $f_{n-\varphi n, \theta^*}$ is the density estimate $f_{n-\varphi n, \theta}$ of smallest index θ^* that minimizes

$$\Delta_{\theta} = \sup_{A \in \mathcal{A}_{\theta}} \left| \int_A f_{n-\varphi n, \theta}(A) - \mu_{\varphi n}(A) \right|$$

where $\mu_{\varphi n}$ is the empirical measure of the validation set $X_{n-\varphi n+1}, \dots, X_n$.

Minimum Distance Estimation (MDE)

Let Θ be the set of the number of splits such that $\Theta := \{0, \dots, \bar{m}_n - 1\}$ where $\bar{m}_n - 1$ is the maximum number of splits allowed.

Every time a split happens during `SplitMostCounts`,

- ▶ Obtain the Yatracos class for the current split θ ;

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The candidate estimate that minimizes Δ_θ is the minimum distance estimate.

└ Minimum Distance Estimation

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- ▶ Need to track statistics for both the training and validation data - recursively computable statistics for validation data;

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Setting up MDE

- ▶ Need to track statistics for both the training and validation data - recursively computable statistics for validation data;
- ▶ Get the Yatracos class for the current Θ - use the RP as a collator (via non-minimal union) to track and compare the histogram estimate at each leaf box of each candidate.

Recursively Computable Statistics for Validation Data

- ▶ The training data $\mathcal{T} := \{x_1, \dots, x_{n-\varphi n}\}$ drive the randomized priority queue RPQ to form an SRP s .
- ▶ The validation data $\mathcal{V} := \{x_{n-\varphi n+1}, \dots, x_n\}$ trickle through s and stay in the boxes of s that contain the data.

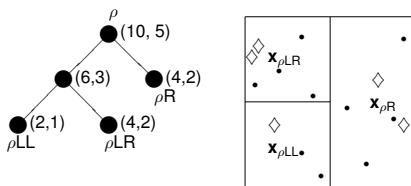


Figure : An SRP s with training (\bullet) and validation data (\diamond) and their respective sample counts ($\#x_{\rho_V}, \#x_{\rho_V}$) that are updated recursively as data fall through the nodes of s .

Recursively Computable Statistics for Validation Data

MDE requires the histogram estimate from the training data and the empirical mass of the validation data:

Histogram estimate obtained from the set of training data

$$f_{n-\varphi n}(\rho V) = \frac{\#\mathbf{x}_{\rho V}}{n \cdot \text{vol}(\mathbf{x}_{\rho V})} .$$

The empirical measure of the validation data

$$\mu_{\varphi n}(\mathbf{x}_{\rho V}) = \frac{\check{\#\mathbf{x}_{\rho V}}}{\varphi n} .$$

Recursively Computable Statistics for Validation Data

The training data and the empirical mass of the validation data can be tracked as $(f_{n-\varphi n, \theta}(\rho V), \mu_{\varphi n}(\mathbf{x}_{\rho V}))$ at each leaf node.

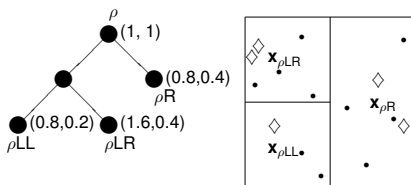


Figure : Tracking the histogram estimate and empirical mass at each node of an SRP s built from a unit square.

RP as a Collator

- ▶ Need to compare the estimates between each SRP $s^{(i)}, 1 < i < \infty$.
- ▶ An efficient way to approach this is to collate these histograms onto an *collator regular paving* or *CRP* where the space of CRP is also $\mathbb{S}_{0:\infty}$.
- ▶ Consider two SRPs $s^{(\theta)}$ and $s^{(\theta')}$ that have the same mother box and for which the corresponding histogram estimates $f_{n,s^{(\theta)}}$ and $f_{n,s^{(\theta')}}$ are computed.
- ▶ By collating the two SRPs we get a CRP c that stores $f_{n,s^{(\theta)}}$ and $f_{n,s^{(\theta')}}$ for each node ρv of c , such that each node ρv has a vector $\mathbf{f}_{n,c}(\rho v) := (f_{n,s^{(\theta)}}(\rho v), f_{n,s^{(\theta')}}(\rho v))$.

RP as a Collator

Collating two SRPs $s^{(\theta)}$ and $s^{(\theta')}$ with the same root box \mathbf{x}_ρ :

Figure : Make the SRP $s^{(\theta)}$ into a CRP c .

$s^{(\theta)}$ with box \mathbf{x}_ρ

$f_{n,s^{(\theta)}}(\rho\text{LR})$	$f_{n,s^{(\theta)}}(\rho\text{R})$
$f_{n,s^{(\theta)}}(\rho\text{LL})$	

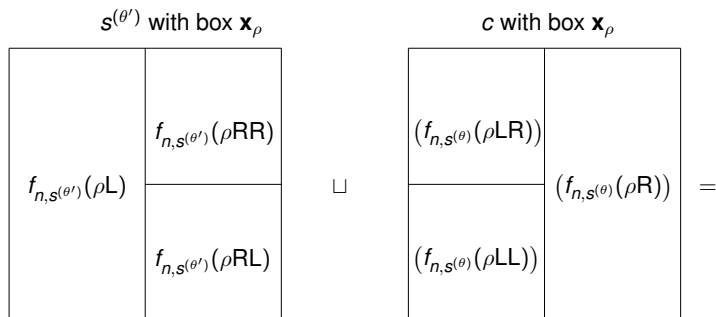
c with box \mathbf{x}_ρ

$(f_{n,s^{(\theta)}}(\rho\text{LR}))$	$(f_{n,s^{(\theta)}}(\rho\text{R}))$
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Collating two SRPs $s^{(\theta)}$ and $s^{(\theta')}$ with the same root box \mathbf{x}_ρ :

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$\begin{pmatrix} f_{n,s^{(\theta)}}(\rho\text{LR}) \\ f_{n,s^{(\theta')}}(\rho\text{L}) \end{pmatrix}$	$\begin{pmatrix} f_{n,s^{(\theta)}}(\rho\text{R}) \\ f_{n,s^{(\theta')}}(\rho\text{RR}) \end{pmatrix}$
$\begin{pmatrix} f_{n,s^{(\theta)}}(\rho\text{LL}) \\ f_{n,s^{(\theta')}}(\rho\text{L}) \end{pmatrix}$	$\begin{pmatrix} f_{n,s^{(\theta)}}(\rho\text{R}) \\ f_{n,s^{(\theta')}}(\rho\text{RL}) \end{pmatrix}$

Minimum Distance Estimation (MDE): An Example

First candidate: $s_0, \theta = 0$.

Second candidate: $s_{1,1}, \theta = 1$.

So $\Theta = \Theta_1 = \{0, 1\}$.

Collate the two candidates:

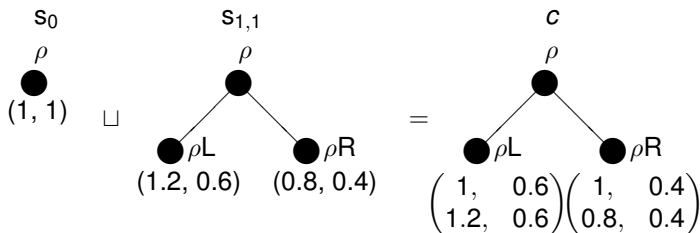
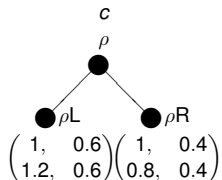


Figure : Collating s_0 and $s_{1,1}$.

Minimum Distance Estimation (MDE): An Example

Compare $f_{n-\varphi n, \theta}$, $\theta \in \Theta$ for each leaf box $\mathbf{x}_{\rho_V} \in \ell(c)$.



At $\mathbf{x}_{\rho L}$,

$$f_{n-\varphi n, \theta=0}(\mathbf{x}_{\rho L}) = 1 < f_{n-\varphi n, \theta=1}(\mathbf{x}_{\rho L}) = 1.2 .$$

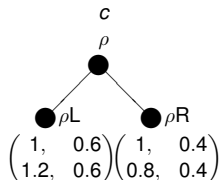
But,

$$f_{n-\varphi n, \theta=1}(\mathbf{x}_{\rho L}) > f_{n-\varphi n, \theta=0}(\mathbf{x}_{\rho L}) .$$

Thus $A_{\theta=1, \theta'=0} = \{\mathbf{x}_{\rho L}\}$ and is in the Yatracos class A_{Θ_1} .

Minimum Distance Estimation (MDE): An Example

Compare $f_{n-\varphi n, \theta}$, $\theta \in \Theta$ for each leaf box $\mathbf{x}_{\rho V} \in \ell(\mathbf{c})$.



At $\mathbf{x}_{\rho R}$,

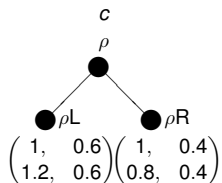
$$f_{n-\varphi n, \theta=0}(\mathbf{x}_{\rho R}) = 1 > f_{n-\varphi n, \theta=1}(\mathbf{x}_{\rho R}) = 0.8 .$$

Thus $A_{\theta=0, \theta'=1} = \{\mathbf{x}_{\rho R}\}$ and is in the Yatracos class A_{Θ_1} .

Finally, we have $\mathcal{A}_{\Theta_1} = \{\mathbf{x}_{\rho L}, \mathbf{x}_{\rho R}\}$.

Minimum Distance Estimation (MDE): An Example

Compare $f_{n-\varphi n, \theta}$, $\theta \in \Theta$ for each leaf box $\mathbf{x}_{\rho v} \in \ell(c)$.



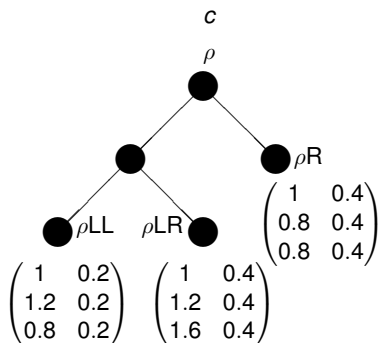
Can also express \mathcal{A}_{Θ_1} in a matrix as follows:

$$\mathcal{A}_{\Theta_1} = \begin{pmatrix} \mathbf{A}_{0,0} & \mathbf{A}_{0,1} \\ \mathbf{A}_{1,0} & \mathbf{A}_{1,1} \end{pmatrix} = \begin{pmatrix} \emptyset & \mathbf{x}_{\rho R} \\ \mathbf{x}_{\rho L} & \emptyset \end{pmatrix}. \quad (1)$$

Note that the diagonal elements are all empty sets because there are no comparisons for the set $\{\theta, \theta'\}$ where $\theta = \theta'$.

Minimum Distance Estimation (MDE): An Example

Make another split at node ρ_L to produce the nodes ρ_{LL} and ρ_{LR} and get the SRP s_{221} . Perform collation to get the following collator c :



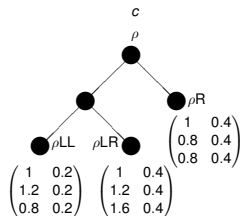
Minimum Distance Estimation (MDE): An Example

Current Θ is now $\Theta = \{0, 1, 2\}$. To update the Yatracos class:

- ▶ Denote $\mathbf{x}_{\rho V}^*$ as the leaf box that is being split currently.
- ▶ Since only one leaf box is split every time, instead of comparing the estimates $f_{n-\varphi n, \theta}(\mathbf{x}_{\rho V})$ at each leaf box, we need only compare the estimates of its sub-boxes $\{\mathbf{x}_{\rho L}^*, \mathbf{x}_{\rho R}^*\}$ to update the Yatracos class.
- ▶ Thus we need not check the estimates at all the leaf boxes.

Minimum Distance Estimation (MDE): An Example

Here $\mathbf{x}_{\rho V}^* = \mathbf{x}_{\rho L}$. Only need to compare the estimates for each θ at the leaf boxes $\mathbf{x}_{\rho LL}$ and $\mathbf{x}_{\rho LR}$.



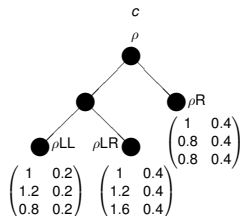
Compare the estimates of the pair $(0, 2)$ at $\mathbf{x}_{\rho LL}$:

$$f_{n-\varphi n, \theta=0}(\mathbf{x}_{\rho LL}) = 1 > f_{n-\varphi n, \theta'=2}(\mathbf{x}_{\rho LL}) = 0.8 .$$

Thus $\mathbf{x}_{\rho LL}$ will be taken into the set $A_{0,2}$.

Minimum Distance Estimation (MDE): An Example

Here $\mathbf{x}_{\rho V}^* = \mathbf{x}_{\rho L}$. Only need to compare the estimates for each θ at the leaf boxes $\mathbf{x}_{\rho LL}$ and $\mathbf{x}_{\rho LR}$.



From $A_{0,1}$ of Equation 1, we also know that $f_{n-\varphi n, \theta=0}(\mathbf{x}_{\rho R})$ is larger than $f_{n-\varphi n, \theta=2}(\mathbf{x}_{\rho R})$. This will also be true for the pair $(0, 2)$. Thus the set $A_{0,2}$ is $\mathbf{x}_{\rho R} \cup \mathbf{x}_{\rho LL}$.

Minimum Distance Estimation (MDE): An Example

- ▶ If $A_{0,1}$ was a box that was split, no unions will be taken with this box since it is no longer a leaf box.
- ▶ In general, at some leaf box \mathbf{x}_{ρ_V} for which its estimates are being compared, for any pair $(\theta, \theta'), \theta \neq \theta'$, if $A_{\theta, \theta'} \neq \{\mathbf{x}_{\rho_V^*}\}$, where $\mathbf{x}_{\rho_V^*}$ was the box being split, we will take the union of \mathbf{x}_{ρ_V} with the elements of the set $A_{\theta-1, \theta'}$.
- ▶ Besides, since the sub-boxes will have the same estimate as its parent box, it will be redundant to make comparisons for the pair $\{0, 1\}$.
- ▶ Therefore instead of doing $\binom{3}{2}$ comparisons, we now only need $\binom{2}{1}$ comparisons, i.e. comparing the estimates at the pairs $\{0, 2\}$ and $\{1, 2\}$.

Minimum Distance Estimation (MDE): An Example

Continue the comparisons for the other sub-box $\mathbf{x}_{\rho LR}$ and for all remaining comparison pairs.

The final Yatracos class \mathcal{A}_{Θ_2} is:

$$\mathcal{A}_{\Theta_2} = \begin{pmatrix} A_{0,0} & A_{0,1} & A_{0,2} \\ A_{1,0} & A_{1,1} & A_{1,2} \\ A_{2,0} & A_{2,1} & A_{2,2} \end{pmatrix} = \begin{pmatrix} \emptyset & \mathbf{x}_{\rho R} & \mathbf{x}_{\rho R} \cup \mathbf{x}_{\rho LL} \\ \mathbf{x}_{\rho L} & \emptyset & \mathbf{x}_{\rho LL} \\ \mathbf{x}_{\rho LR} & \mathbf{x}_{\rho LR} & \emptyset \end{pmatrix} .$$

Minimum Distance Estimation (MDE): An Example

The corresponding Δ_θ values for \mathcal{A}_{Θ_1} and \mathcal{A}_{Θ_2} :

	$\Delta_\theta = \int_{\mathbf{x}_{\rho V}} f_{n-\varphi n} - \mu_{\varphi n}(\mathbf{x}_{\rho V})$	
θ	$\Theta_1 = \{0, 1\}$	$\Theta_2 = \{0, 1, 2\}$
$\theta = 0$	0.1	0.15
$\theta = 1$	0	0.1
$\theta = 2$	-	0

Table : Table of Δ_θ values.

- ▶ Take \mathcal{A}_{Θ_2} to be the final Yatracos class;
- ▶ Observe the column associated with Θ_2 ;
- ▶ The minimum distance estimate $f_{n-\varphi n, \theta^*}$ is the estimate at $\theta = 2$ since $\Delta_{\theta=2}$ is the minimum over all $\theta \in \Theta_2$.

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- ▶ Smoother posterior mean from MCMC samples on the space of adaptive multi-variate histograms with partitions in $\mathbb{S}_{0:\infty}$. NFL: MCMC convergence issues exist!
- ▶ Higher (1000) dimensional densities can be estimated fast and rough (but L_1 -consistent) with the approach especially with `SplitMostCounts` PQ and further decisions can be done with appropriate *mapped RP arithmetic* over $\mathbb{S}_{0:\infty}$.

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Gratitude for Operating Fiscal Environment

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