Approximating the total variation distance between two product distributions

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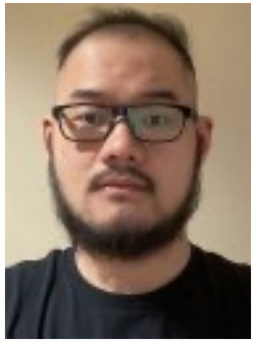
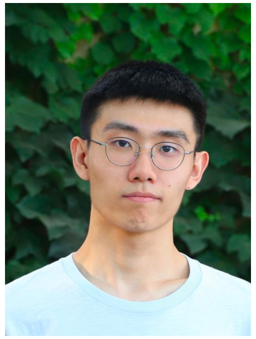
Based on joint works with







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Randomised Algorithm (Heng Guo, Mark Jerrum, Jiaheng Wang)

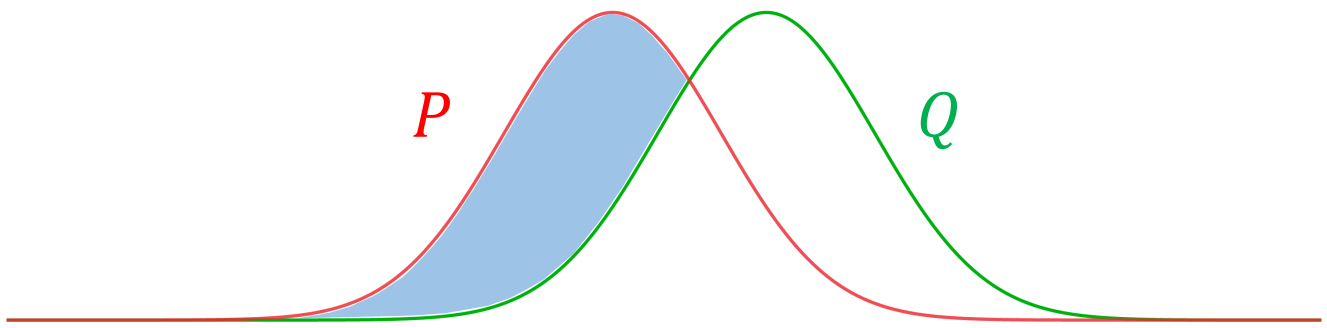
Deterministic Algorithm (Tianren Liu, Liqiang Liu)

Shonan Meeting: MCMC 2.0 Shonan, Japan, Sep 7, 2023

Total Variation distance

Total variation (TV) distance between $\mathbb{P}$ and $\mathbb{Q}$ over state space Ω

$$d_{TV}(\mathbb{P},\mathbb{Q}) = \frac{1}{2}\sum_{x\in\Omega}|\mathbb{P}(x)-\mathbb{Q}(x)| = \max_{S\subseteq\Omega}|\mathbb{P}(S)-\mathbb{Q}(S)|$$



Properties of TV distance

- metric (triangle inequality)
- bounded
- data processing inequality
- various characterisations

Applications of TV distance

- property testing
- Markov chain mixing time
- approximate algorithms
- learning algorithms

Compute TV distance

[Bhattacharyya, Gayen, Meel, Myrisiotis,Pavan, Vinodchandran, 2022]

- **Input:** descriptions of two distributions $\mathbb{P}, \mathbb{Q}$ over Ω
- **Output:** the total variation distance between $\mathbb{P}$ and $\mathbb{Q}$

Trivial algorithm: enumerate all $x \in \Omega$ and add $\frac{1}{2}|\mathbb{P}(x) - \mathbb{Q}(x)|$ together

Challenge:$\mathbb{P}$ and $\mathbb{Q}$ have ***succinct descriptions***

- $|\Omega|$ can be ***exponentially large*** w.r.t. the size of input

Examples: probabilistic graphical models, spin systems.

Product distribution

Product distribution $\mathbb{P}$ over $[s]^n$

$$\mathbb{P} = \mathbb{P}_1 \times \mathbb{P}_2 \times \cdots \times \mathbb{P}_n$$

$$\forall X, \mathbb{P}(X) = \prod_{i=1}^{n} \mathbb{P}_i(X_i)$$

$\mathbb{P}_i$ is a distribution over $[s] = \{1,2,\dots,s\}$

Random sample $X = (X_1, X_2, \dots, X_n) \sim \mathbb{P}$

$X \in [s]^n$: n-dimensional random vector

$X_i \in [s]$: independent sample from $\mathbb{P}_i$

$\mathbb{P}$ can be described by $\{\, \mathbb{P}_i : [s] \to [0,1] \mid 1 \le i \le n \,\}$

description size
sn

state space size
s^n

Compute TV distance between product distributions

[Bhattacharyya, Gayen, Meel, Myrisiotis,Pavan,Vinodchandran, 2022]

- **Input:** distributions $\{\mathbb{P}_i, \mathbb{Q}_i | 1 \leq i \leq n\}$ specifying $\mathbb{P}$ and $\mathbb{Q}$ over $[s]^n$
- **Output:** the total variation distance between $\mathbb{P}$ and $\mathbb{Q}$

Theorem [BGMMPV22]: the problem is **#P-complete** even for Boolean case $(s = 2)$

FPTAS (Full Poly-time Approximation Scheme)

A *deterministic* algorithm outputs a $\hat{d}$ in time $\mathrm{poly}(n, s, 1/\epsilon)$

$$(1-\epsilon)d_{TV}(\mathbb{P}, \mathbb{Q}) \leq \hat{d} \leq (1+\epsilon)d_{TV}(\mathbb{P}, \mathbb{Q})$$

FPRAS (Full Poly-time Randomised Approximation Scheme)

A *randomised* algorithm outputs a random $\hat{d}$ in time $\mathrm{poly}(n, s, 1/\epsilon)$

$$\Pr\left[(1-\epsilon)d_{TV}(\mathbb{P}, \mathbb{Q}) \leq \hat{d} \leq (1+\epsilon)d_{TV}(\mathbb{P}, \mathbb{Q})\right] \geq 2/3$$

Previous results

Theorem [BGMMPV22] ***FPTAS/FPRAS*** exists for product distributions $\mathbb{P}, \mathbb{Q}$ such that

- $\mathbb{P}$ and $\mathbb{Q}$ are *Boolean* distributions ($s = 2$)
- $\mathbb{Q}$ has *constant number* of distinct marginals (e.g. uniform distribution over $\{0,1\}^n$)

Theorem [BGMMPV22] ***FPRAS*** exists for product distributions $\mathbb{P}, \mathbb{Q}$ such that

- $\mathbb{P}$ and $\mathbb{Q}$ are *Boolean* distributions ($s = 2$)
- $\forall i \in [n], \underbrace{\mathbb{P}_i(1) \geq \mathbb{Q}_i(1)}_{\text{break symmetry}}$ and $\underbrace{\mathbb{P}_i(1) \geq 1/2}_{\text{marginal lower bound}}$

Open problem [BGMMPV22]**:**

Do FPTAS/FPRAS exist for ***general*** product distributions?

Our results [F., Guo, Jerrum, Wang 2023] [F., Liu, Liu 2023] **:**

FPTAS/FPRAS exist for ***general*** product distributions

Product distributions $\mathbb{P}, \mathbb{Q}$ over $[s]^n$ and error bound $0 < \epsilon < 1$

- FPTAS running time: $\tilde{O}\left(\frac{sn^2}{\epsilon}\log\frac{1}{d_{TV}(\mathbb{P},\mathbb{Q})}\right)$
- FPRAS running time : $\tilde{O}\left(\frac{sn^2}{\epsilon^2}\right)$

Extension: Markov chains [F., Liu, Liu 2023]

- distributions π_1, π_2 and transition Matrices M_1, M_2 over state space $[s]$
- approximate $d_{TV}((X_k)_{k=1}^n, (Y_k)_{k=1}^n)$ such that
  - $X_1 \sim \pi_1$ and $X_k \sim M_1(X_{k-1},\cdot)$ / $Y_1 \sim \pi_2$ and $Y_k \sim M_2(Y_{k-1},\cdot)$

FPTAS exists for TV-distance between Markov chains

A natural estimator

Total variation (TV) distance between $\mathbb{P}$ and $\mathbb{Q}$ over state space Ω

$$d_{TV}(\mathbb{P},\mathbb{Q}) = \frac{1}{2}\sum_{x\in\Omega} |\mathbb{P}(x) - \mathbb{Q}(x)| = \sum_{x\in\Omega:\mathbb{Q}(X)>\mathbb{P}(X)} |\mathbb{Q}(x) - \mathbb{P}(x)| = \sum_{x\in\Omega:\mathbb{Q}(X)>\mathbb{P}(X)} \mathbb{Q}(X)\left(1 - \frac{\mathbb{P}(X)}{\mathbb{Q}(X)}\right)$$

Ratio $R \sim \mathbb{R} = (\mathbb{P}||\mathbb{Q})$

$$R = \frac{\mathbb{P}(X)}{\mathbb{Q}(X)}, \qquad \text{where } X \sim \mathbb{Q}$$

$$d_{TV}(\mathbb{P},\mathbb{Q}) = \mathbb{E}[\max(0,1-R)]$$

- sample R independent
- take average of $\max(0,1-R)$

unbiased estimator of $d_{TV}(\mathbb{P},\mathbb{Q})$

- Approximate the TV distance with ***additive*** error $\hat{d} \in d_{TV}(\mathbb{P},\mathbb{Q}) \pm \epsilon$
- ***Relative-error*** approximation requires many samples because

<u>$d_{TV}(\mathbb{P},\mathbb{Q})$ can be exponentially small</u>

TV distance and coupling

- **Distributions**: $\mathbb{P}$ and $\mathbb{Q}$ over the domain Ω
- **Coupling**: a joint $(X, Y) \in \Omega \times \Omega$ such that $X \sim \mathbb{P}$ and $Y \sim \mathbb{Q}$

Coupling Inequality (Coupling Lemma)

$$\forall \text{coupling } (X, Y), \qquad d_{TV}(\mathbb{P}, \mathbb{Q}) \leq \Pr[X \neq Y]$$

$$\exists \text{optimal coupling } (X, Y), \qquad d_{TV}(\mathbb{P}, \mathbb{Q}) = \Pr[X \neq Y]$$

The optimal coupling may ***not*** be unique

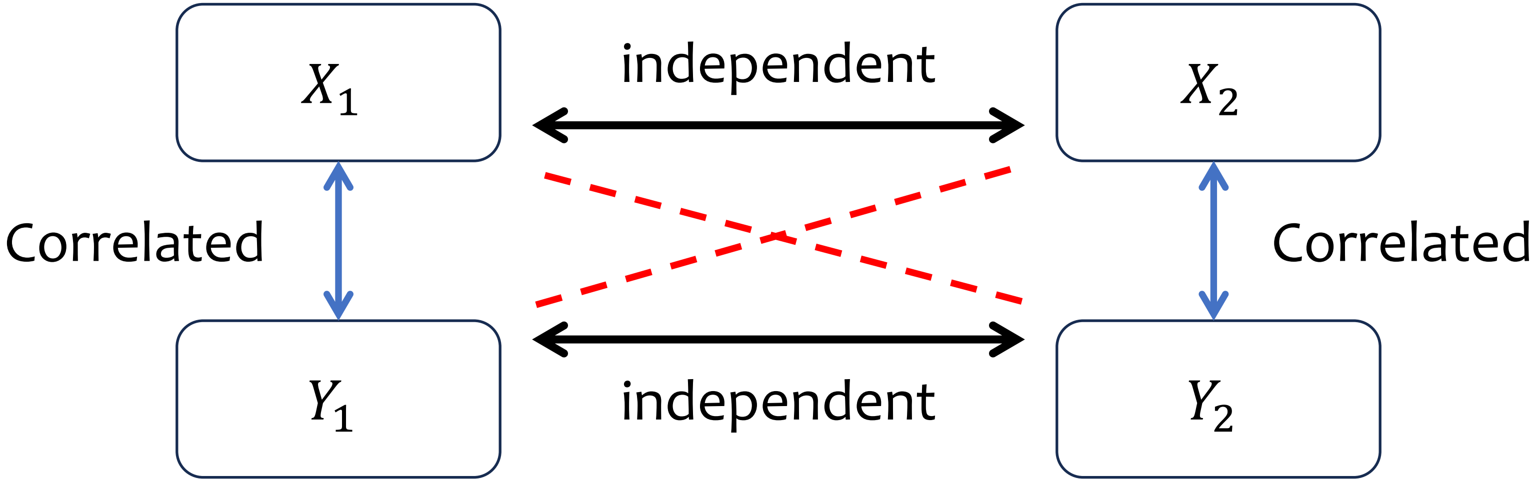
Given two **product distributions** $\mathbb{P}, \mathbb{Q}$ over $[s]^n$,

what is their optimal coupling?

A ***greedy*** coupling $(X, Y) = ((X_1, X_2, \dots, X_n), (Y_1, Y_2, \dots, Y_n))$ of $\mathbb{P}, \mathbb{Q}$

each (X_i, Y_i) is coupled ***optimally*** and ***independently***

- Greedy coupling is **not** an optimal coupling



Optimal coupling can utilise the correlations of (X_1, Y_2) and (Y_1, X_2)

A ***greedy*** coupling $(X,Y)=((X_1,X_2,\dots,X_n),(Y_1,Y_2,\dots,Y_n))$ of $\mathbb{P},\mathbb{Q}$

each (X_i,Y_i) is coupled ***optimally*** and ***independently***

- Greedy coupling is **not** an optimal coupling
- Greedy coupling can **approximate** the optimal coupling

$$d_{TV}(\mathbb{P},\mathbb{Q}) \le \Pr_{\text{Greedy}}[X \ne Y] \le n d_{TV}(\mathbb{P},\mathbb{Q})$$

Proof.

$$\Pr_{\text{Greedy}}[X \ne Y] \le \sum_{i=1}^{n} \Pr[X_i \ne Y_i] = \sum_{i=1}^{n} d_{TV}(\mathbb{P}_i,\mathbb{Q}_i) \le n d_{TV}(\mathbb{P},\mathbb{Q})$$

local optimal coupling

A ***greedy*** coupling $(X,Y) = ((X_1, X_2, \dots, X_n), (Y_1, Y_2, \dots, Y_n))$ of $\mathbb{P}, \mathbb{Q}$

each (X_i, Y_i) is coupled ***optimally*** and ***independently***

- Greedy coupling is **not** an optimal coupling
- Greedy coupling can **approximate** the optimal coupling

$$d_{TV}(\mathbb{P}, \mathbb{Q}) \le \Pr_{\text{greedy}}[X \ne Y] \le n d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Discrepancy of greedy coupling can be computed ***efficiently***

$$\Pr_{\text{greedy}}[X \ne Y] = 1 - \Pr_{\text{greedy}}[X = Y] = 1 - \prod_{i=1}^{n} \left(1 - d_{TV}(\mathbb{P}_i, \mathbb{Q}_i)\right)$$

- Our ideal: estimate $\frac{\Pr_{\text{opt}}[X \ne Y]}{\Pr_{\text{greedy}}[X \ne Y]} = \frac{d_{TV}(\mathbb{P}, \mathbb{Q})}{\Pr_{\text{greedy}}[X \ne Y]} \ge \frac{1}{n}$

Our Estimator [F., Guo, Jerrum, Wang 2023]

- π: the distribution of X in the greedy coupling conditional on $X \neq Y$
$$\forall \sigma \in [s]^n, \qquad \pi(\sigma) = \Pr_{\text{greedy}}[X = \sigma \mid X \neq Y]$$
- f: a function $[s]^n \to \mathbb{R}_{>0}$ such that
$$\forall \sigma \in [s]^n, \qquad f(\sigma) = \frac{\Pr_{\text{opt}}[X = \sigma \wedge X \neq Y]}{\Pr_{\text{greedy}}[X = \sigma \wedge X \neq Y]} = \frac{\max\{0, \mathbb{P}(\sigma) - \mathbb{Q}(\sigma)\}}{\Pr_{\text{greedy}}[X = \sigma \wedge X \neq Y]}$$
- Estimator: $f(\sigma)$ where $\sigma \sim \pi$

Properties of the estimator

- **Correct expectation**
$$\mathbb{E}_{\sigma\sim\pi}[f(\sigma)] = \frac{\Pr_{\text{opt}}[X \neq Y]}{\Pr_{\text{greedy}}[X \neq Y]} = \frac{d_{TV}(\mathbb{P}, \mathbb{Q})}{\Pr_{\text{greedy}}[X \neq Y]} \geq \frac{1}{n}$$
- **Low variance**
$$\mathrm{Var}_{\sigma\sim\pi}[f(\sigma)] \leq 1$$

$$\forall \sigma \in [s]^V, \qquad \Pr_{\text{opt}}[X = \sigma \wedge X \neq Y] \leq \Pr_{\text{greedy}}[X = \sigma \wedge X \neq Y]$$

⇒

$$\forall \sigma \in [s]^V, \qquad 0 \leq f(\sigma) \leq 1$$

Our Estimator [F., Guo, Jerrum, Wang 2023]

- π: the distribution of X in the greedy coupling conditional on $X \neq Y$

$$\forall \sigma \in [s]^n, \qquad \pi(\sigma) = \Pr_{\text{greedy}}[X = \sigma \mid X \neq Y]$$

- f: a function $[s]^V \to \mathbb{R}_{>0}$ such that

$$\forall \sigma \in [s]^n, \qquad f(\sigma) = \frac{\Pr_{\text{opt}}[X = \sigma \wedge X \neq Y]}{\Pr_{\text{greedy}}[X = \sigma \wedge X \neq Y]} = \frac{\max\{0, \mathbb{P}(\sigma) - \mathbb{Q}(\sigma)\}}{\Pr_{\text{greedy}}[X = \sigma \wedge X \neq Y]}$$

- Estimator: $f(\sigma)$ where $\sigma \sim \pi$

Properties of the estimator

- **Correct expectation**

$$\mathbb{E}_{\sigma\sim\pi}[f(\sigma)] = \frac{\Pr_{\text{opt}}[X \neq Y]}{\Pr_{\text{greedy}}[X \neq Y]} = \frac{d_{TV}(\mathbb{P}, \mathbb{Q})}{\Pr_{\text{greedy}}[X \neq Y]} = R \geq \frac{1}{n}$$

- **Low variance**

$$\mathrm{Var}_{\sigma\sim\pi}[f(\sigma)] \leq 1$$

- **Efficient computation**
  - a random sample of $\sigma \sim \pi$ can be generated in time $O(n)$
  - given any $\sigma \in \{0,1\}^n$, $f(\sigma)$ can be computed in time $O(n)$

$O\left(\frac{n}{\epsilon^2}\right)$ samples

Sampling algorithm for the distribution π:

$$\forall \sigma \in [s]^n, \qquad \pi(\sigma) = \Pr_{\text{greedy}}[X = \sigma \mid X \neq Y]$$

- The greedy coupling is a product distribution
- The condition $X \neq Y$ is not complicated

Algorithm

- Sample $\sigma \in [s]^V$ index by index;
- Conditional on $\sigma_1, \sigma_2, \dots, \sigma_{i-1}$, ***exactly*** compute the marginal of σ_i and sample

$$\Pr[\sigma_1 = c] = \Pr[\, X_1 = c \mid X \neq Y \,] = \frac{\Pr[\, X \neq Y \mid X_1 = c\,] \cdot \Pr[X_1 = c]}{\Pr[X \neq Y]}$$

- ✅ $\Pr[X_1 = c] = P_1(c)$
- ✅ $\Pr[X \neq Y] = 1 - \Pr[X = Y] = 1 - \prod_{i=1}^{n}(1 - d_{TV}(P_i, Q_i))$
- ✅ $\Pr[X \neq Y | X_1 = c] = 1 - \Pr[\, X = Y \mid X_1 = c \,]$

Sampling algorithm for the distribution π:

$$\forall \sigma \in [s]^n, \qquad \pi(\sigma) = \Pr_{\text{greedy}}[X = \sigma \mid X \neq Y]$$

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$$\Pr[\sigma_1 = c] = \Pr[X_1 = c \mid X \neq Y] = \frac{\Pr[X \neq Y \mid X_1 = c] \cdot \Pr[X_1 = c]}{\Pr[X \neq Y]}$$

☑ $\Pr[X_1 = c] = P_1(c)$

☑ $\Pr[X \neq Y] = 1 - \Pr[X = Y] = 1 - \prod_{i=1}^{n}(1 - d_{TV}(P_i, Q_i))$

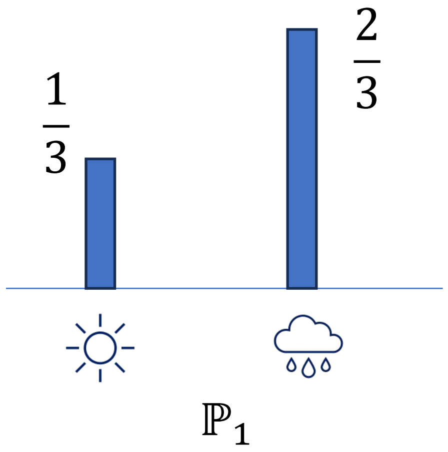
☑ $\Pr[X \neq Y | X_1 = c] = 1 - \Pr[X = Y \mid X_1 = c] = 1 - \Pr[X_1 = Y_1 \mid X_1 = c] \prod_{i=2}^{n} \Pr[X_i = Y_i]$

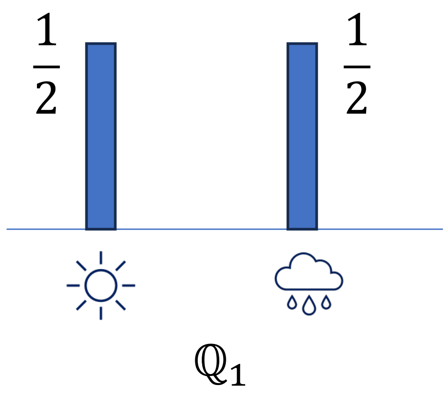
Ratio and deterministic algorithm

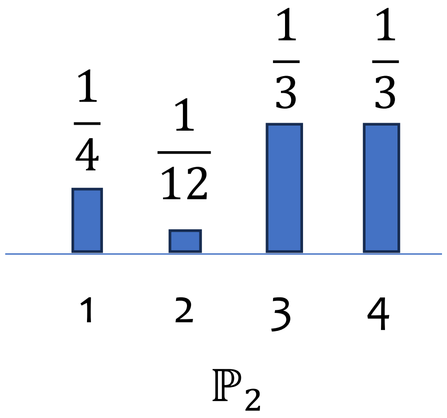
Ratio $R \sim \mathbb{R} = (\mathbb{P}||\mathbb{Q})$

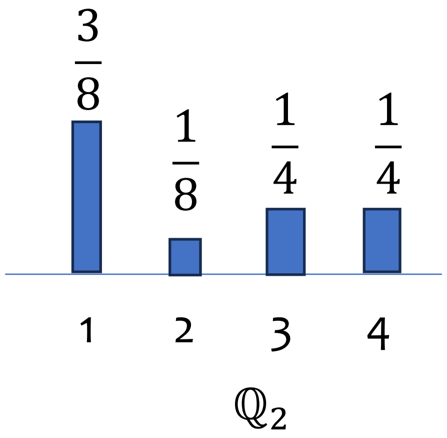
$$R = \frac{\mathbb{P}(X)}{\mathbb{Q}(X)}, \qquad \text{where } X \sim Q$$

$$d_{TV}(\mathbb{P},\mathbb{Q}) = d_{TV}(\mathbb{R}) = \mathbb{E}[\max(0,1-R)]$$



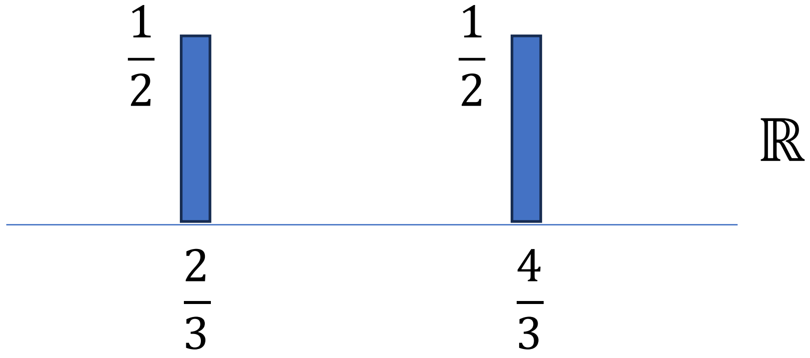






$$\mathbb{R} = (\mathbb{P}_1||\mathbb{Q}_1) = (\mathbb{P}_2||\mathbb{Q}_2)$$

$$d_{TV}(\mathbb{R}) = d_{TV}(\mathbb{P}_1,\mathbb{Q}_1) = d_{TV}(\mathbb{P}_2,\mathbb{Q}_2) = \frac{1}{6}$$



Ratio and deterministic algorithm

Ratio $R \sim \mathbb{R} = (\mathbb{P}||\mathbb{Q})$

$$R = \frac{\mathbb{P}(X)}{\mathbb{Q}(X)}, \qquad \text{where } X \sim Q$$

$$d_{TV}(\mathbb{P}, \mathbb{Q}) = d_{TV}(\mathbb{R}) = \mathbb{E}[\max(0, 1 - R)]$$

$\mathbb{R}$ ***preserves*** $d_{TV}(\mathbb{P}, \mathbb{Q})$, may compress some redundant information

If $\mathbb{R}_1 = (\mathbb{P}_1||\mathbb{Q}_1)$ and $\mathbb{R}_2 = (\mathbb{P}_2||\mathbb{Q}_2)$, then

$$\mathbb{R}_1 \cdot_{\text{ind}} \mathbb{R}_2 = (\mathbb{P}_1 \times \mathbb{P}_2 || \mathbb{Q}_1 \times \mathbb{Q}_2)$$

- $\mathbb{P}_1 \times \mathbb{P}_2$ is the **product distribution** $\mathbb{P}_1$ and $\mathbb{P}_2$
- $\mathbb{R}_1 \cdot_{\text{ind}} \mathbb{R}_2$ is the distribution of the **product of two independent random real number**

$$R_1 R_2 \sim \mathbb{R}_1 \cdot_{\text{ind}} \mathbb{R}_2, \ \text{where } R_1 \sim \mathbb{R}_1 \text{ and } R_2 \sim \mathbb{R}_2 \text{ are ind. samples}$$

A naïve deterministic algorithm

- **Input**: distributions of $\mathbb{P}_1, \mathbb{P}_2, \ldots, \mathbb{P}_n, \mathbb{Q}_1, \mathbb{Q}_2, \ldots, \mathbb{Q}_n$ and an error bound ϵ
- **Output**: an approximation of $d_{TV}(\mathbb{P}, \mathbb{Q})$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- Compute $\mathbb{R}_{1:1} \leftarrow \mathbb{R}_1$
- Compute $\mathbb{R}_{1:2} \leftarrow \mathbb{R}_{1:1} \cdot_{ind} \mathbb{R}_2$

…

- Compute $\mathbb{R}_{1:i} \leftarrow \mathbb{R}_{1:i-1} \cdot_{ind} \mathbb{R}_i$

…

- Compute distribution $\mathbb{R}_{1:n} \leftarrow \mathbb{R}_{1:n-1} \cdot_{ind} \mathbb{R}_n$
- Return $d_{TV}(\mathbb{R}_{1:n}) = \mathbb{E}_{R \sim \mathbb{R}_{1:n}}[\max(0,1-R)]$

Exact computing of $d_{TV}(\mathbb{P}, \mathbb{Q})$

The support size is ***large***

$$|\text{supp}(\mathbb{R}_{1:i})| = \exp(\Omega(i))$$

Efficiently compute $\widehat{\mathbb{R}}_{\mathbf{1:n}}$ s.t.

$$d_{TV}\left(\widehat{\mathbb{R}}_{1:\boldsymbol{n}}\right) \approx d_{TV}(\mathbb{R}_{1:n})$$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:2})$

…
- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{1:i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:i})$

…

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{1:n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:n})$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R\sim\widehat{\mathbb{R}}_{1:n}}[\max(0,1-R)]$

$$\widehat{\mathbb{R}} \leftarrow \text{Sparsify}(\mathbb{R}')$$

- The support size of $\widehat{\mathbb{R}}$ is small
- $\widehat{\mathbb{R}}$ and $\mathbb{R}'$ is close with respect to a ***metric*** $\Delta(\cdot,\cdot)$

- If $\mathbb{R}_1 \approx \mathbb{R}_2$, then $d_{TV}(\mathbb{R}_1) \approx d_{TV}(\mathbb{R}_2)$

$$|d_{TV}(\mathbb{R}_1) - d_{TV}(\mathbb{R}_2)| \leq \Delta(\mathbb{R}_1, \mathbb{R}_2)$$

- If $\mathbb{R}_1 \approx \mathbb{R}_2$ and $\mathbb{R}_3 \approx \mathbb{R}_4$, then $\mathbb{R}_1 \cdot_{ind} \mathbb{R}_3 \approx \mathbb{R}_2 \cdot_{ind} \mathbb{R}_4$

$$\Delta(\mathbb{R}_1 \cdot_{ind} \mathbb{R}_3, \mathbb{R}_2 \cdot_{ind} \mathbb{R}_4) \leq \Delta(\mathbb{R}_1, \mathbb{R}_2) + \Delta(\mathbb{R}_3, \mathbb{R}_4)$$

$$\Delta(\mathbb{R}_1, \mathbb{R}_2) = \min\left\{ d_{TV}(\mathbb{P}_1, \mathbb{P}_2) + d_{TV}(\mathbb{Q}_1, \mathbb{Q}_2) \;\middle|\; \substack{\mathbb{R}_1 = (\mathbb{P}_1 || \mathbb{Q}_1) \\ \mathbb{R}_2 = (\mathbb{P}_2 || \mathbb{Q}_2)} \right\}$$

minimum total variation distance

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

$$\mathbb{R}_{i:n} = \mathbb{R}_i \cdot \mathbb{R}_{i+1} \cdot \ldots \cdot \mathbb{R}_n$$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

$$\Delta\left(\widehat{\mathbb{R}}_{1:1}, \mathbb{R}_1\right) = 0 \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:2})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:2}, \widehat{\mathbb{R}}_{1:1} \cdot \mathbb{R}_2\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

…

- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:i})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:i}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

…

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:n})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:n}, \widehat{\mathbb{R}}_{1:n-1} \cdot \mathbb{R}_n\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R \sim \widehat{\mathbb{R}}_{1:n}}[\max(0, 1 - R)]$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:2})$

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- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:i})$

…

$\Delta\left(\widehat{\mathbb{R}}_{1:i} \cdot \mathbb{R}_{i+1:n}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i \cdot \mathbb{R}_{i+1:n}\right)$

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:n})$

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- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:2})$

…

- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:i})$

…

$$\Delta\left(\widehat{\mathbb{R}}_{1:i} \cdot \mathbb{R}_{i+1:n}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i \cdot \mathbb{R}_{i+1:n}\right)$$
$$\leq \Delta\left(\widehat{\mathbb{R}}_{1:i}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i\right) + \Delta\left(\mathbb{R}_{i+1:n}, \mathbb{R}_{i+1,n}\right)$$
$$\leq 0 + \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow \textbf{Sparsify}(\mathbb{R}'_{1:n})$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R \sim \widehat{\mathbb{R}}_{1:n}}[\max(0,1 - R)]$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

$$\Delta\left(\widehat{\mathbb{R}}_{1:1} \cdot \mathbb{R}_{2:n}, \mathbb{R}_{1:n}\right) \le \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:2})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:2} \cdot \mathbb{R}_{3:n}, \widehat{\mathbb{R}}_{1:1} \cdot \mathbb{R}_{2:n}\right) \le \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

…

- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:i})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:i} \cdot \mathbb{R}_{i+1:n}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_{i:n}\right) \le \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

…

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:n})$

$$\Delta\left(\widehat{\mathbb{R}}_{1:n}, \widehat{\mathbb{R}}_{1:n-1} \cdot \mathbb{R}_n\right) \le \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R \sim \widehat{\mathbb{R}}_{1:n}}[\max(0,1-R)]$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:2})$

…

- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:i})$

…

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:n})$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R \sim \widehat{\mathbb{R}}_{1:n}}[\max(0, 1 - R)]$

$$\Delta\left(\widehat{\mathbb{R}}_{1:1} \cdot \mathbb{R}_{2:n}, \mathbb{R}_{1:n}\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

$$\Delta\left(\widehat{\mathbb{R}}_{1:2} \cdot \mathbb{R}_{3:n}, \widehat{\mathbb{R}}_{1:1} \cdot \mathbb{R}_{2:n}\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

$$\Delta\left(\widehat{\mathbb{R}}_{1:i} \cdot \mathbb{R}_{i+1:n}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_{i:n}\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

$$\Delta\left(\widehat{\mathbb{R}}_{1:n}, \widehat{\mathbb{R}}_{1:n-1} \cdot \mathbb{R}_n\right) \leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

- Compute $\mathbb{R}_i \leftarrow (\mathbb{P}_i || \mathbb{Q}_i)$ for all $i \in [n]$

- $\widehat{\mathbb{R}}_{1:1} \leftarrow \mathbb{R}_1$

- Compute $\mathbb{R}'_{1:2} \leftarrow \widehat{\mathbb{R}}_{1:1} \cdot_{ind} \mathbb{R}_2$
- $\widehat{\mathbb{R}}_{1:2} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:2})$

…

- Compute $\mathbb{R}'_{1:i} \leftarrow \widehat{\mathbb{R}}_{i-1} \cdot_{ind} \mathbb{R}_i$
- $\widehat{\mathbb{R}}_{1:i} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:i})$

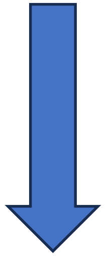
…

- Compute $\mathbb{R}'_{1:n} = \widehat{\mathbb{R}}_{n-1} \cdot_{ind} \mathbb{R}_n$
- $\widehat{\mathbb{R}}_{1:n} \leftarrow$ **Sparsify**$(\mathbb{R}'_{1:n})$

- Return $d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) = \mathbb{E}_{R\sim\widehat{\mathbb{R}}_{1:n}}[\max(0,1-R)]$

By **triangle-inequality** of metric

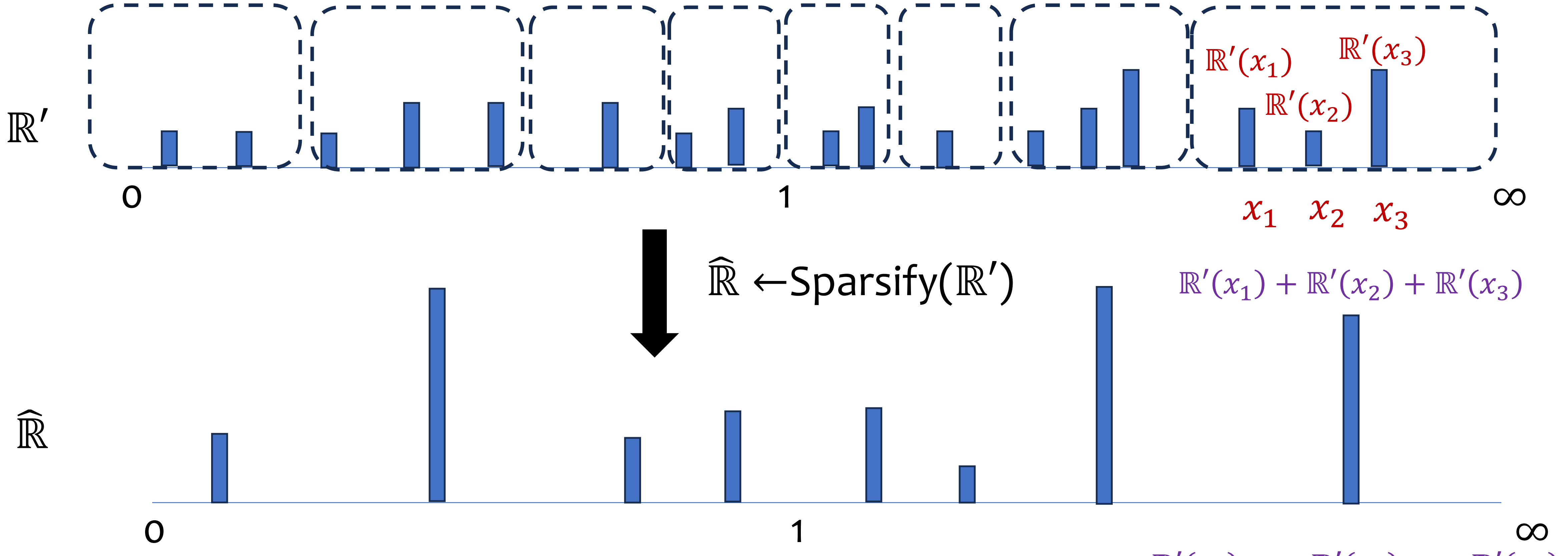
$$\Delta\left(\mathbb{R}_{1:n}, \widehat{\mathbb{R}}_{1:n}\right) \leq \epsilon d_{TV}(\mathbb{P}, \mathbb{Q})$$



$$\mathbb{R}_{1:n} = (\mathbb{P}||\mathbb{Q})$$
$$d_{TV}(\mathbb{R}_{1:n}) = d_{TV}(\mathbb{P}, \mathbb{Q})$$

$$\left|d_{TV}\left(\widehat{\mathbb{R}}_{1:n}\right) - d_{TV}(\mathbb{P}, \mathbb{Q})\right| \leq \epsilon d_{TV}(\mathbb{P}, \mathbb{Q})$$

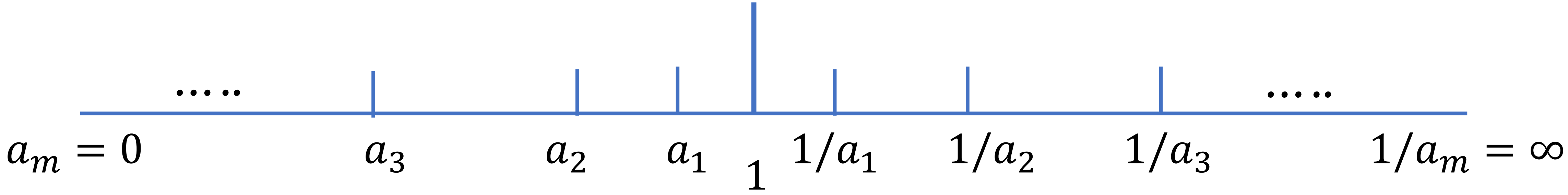
The Sparsify subroutine



$$\frac{x_1\mathbb{R}'(x_1) + x_2\mathbb{R}'(x_2) + x_3\mathbb{R}'(x_3)}{\mathbb{R}'(x_1) + \mathbb{R}'(x_2) + \mathbb{R}'(x_3)}$$

$$= \mathbb{E}_{R' \sim \mathbb{R}'}[R' \mid R' \in I]$$

- Partition $[0, \infty)$ into a set of intervals $\mathcal{I}$
- For each interval $I \in \mathcal{I}$, merge all elements in I into one element



Partition of [0,1]

$$\left\{ \begin{array}{c} [a_1, a_0 = 1) \\ [a_2, a_1) \\ [a_3, a_2) \\ \dots \\ [a_m = 0, a_{m-1}) \end{array} \right.$$

- The first interval is small

$$1 - a_1 \le \delta_s$$

- The length of $[a_i, a_{i-1}]$ is small w.r.t. $1 - a_{i-1}$

$$\forall i > 1, \qquad |a_i - a_{i-1}| \le \epsilon_s \cdot |1 - a_{i-1}|$$

Partition of $(1, \infty)$

$$\left\{ \begin{array}{c} [a_0 = 1, 1/a_1) \\ [1/a_1, 1/a_2) \\ [1/a_2, 1/a_3) \\ \dots \\ [1/a_{m-1}, 1/a_m = \infty) \end{array} \right.$$

$$m = O\left(\frac{1}{\epsilon_s} \log \frac{1}{\delta_s}\right)$$

Error of Sparsification [F., Liu, Liu 2023]

$\mathbb{R} \leftarrow$Sparsify($\mathbb{R}'$) $\Rightarrow$ $\Delta(\mathbb{R}, \mathbb{R}') \leq \epsilon_s d_{TV}(\mathbb{R}') + \delta_s$

- δ_s: ***absolute error*** from merging $[a_1, 1]$ and $\left(1, \frac{1}{a_1}\right)$
- ϵ_s: ***relative error*** from merging other intervals

$$\frac{\epsilon d_{TV}(\mathbb{P}, \mathbb{Q})}{2n^2} \leq \delta_s \leq \frac{\epsilon d_{TV}(\mathbb{P}, \mathbb{Q})}{2n}$$

$$\epsilon_s = \frac{\epsilon}{2n}$$

Merge error in every iteration

$$\Delta\left(\widehat{\mathbb{R}}_{1:i}, \widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i\right)$$

$$\leq \frac{\epsilon}{2n} d_{TV}\left(\widehat{\mathbb{R}}_{1:i-1} \cdot \mathbb{R}_i\right) + \frac{d_{TV}(\mathbb{P}, \mathbb{Q})}{2n}$$

$$\leq \frac{\epsilon}{n} d_{TV}(\mathbb{P}, \mathbb{Q})$$

$$m = O\left(\frac{n}{\epsilon} \log \frac{1}{d_{TV}(\mathbb{P}, \mathbb{Q})}\right)$$

Summary

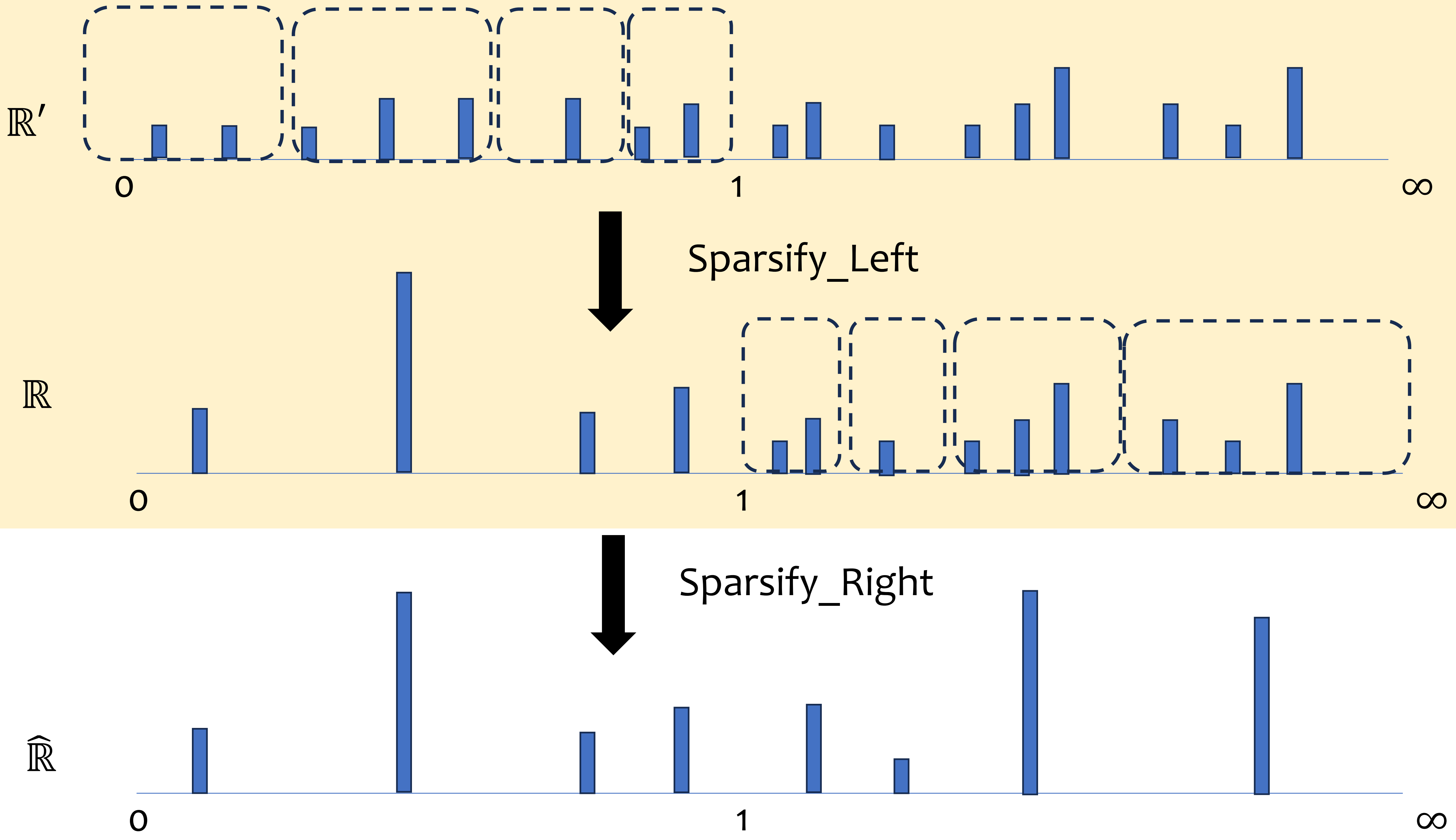
- **Problem:** Compute the TV distance between two ***product distributions***
- **Algorithms:** FPTAS and FPRAS
- **Extension:** TV distance between two ***Markov chains***

Open problems

- ***Better running time*** of FPTAS: remove $\log \frac{1}{d_{TV}(\mathbb{P},\mathbb{Q})}$ in $\tilde{O}(n^2 \log \frac{1}{d_{TV}(\mathbb{P},\mathbb{Q})})$?
- Algorithm/complexity for approximating TV distance of ***general models***
  - Graphical models
  - Hidden Markov chains
- Relation between ***approximating TV distance*** and ***sampling/counting***

Appendix

Analysis of the sparsification error



ℝ′
0
1
∞
Sparsify_Left
ℝ
0
1
∞
Sparsify_Right
ℝ̂
0
1
∞

$\mathbb{R} \leftarrow$ **Sparsify_Left**$(\mathbb{R}')$ merge intervals $\mathcal{I} = \{[a_1, a_0), [a_2, a_1), \ldots, [a_m, a_{m-1})\}$

$\mathbb{R}' = (\mathbb{P}' || \mathbb{Q}')$, where $\mathbb{Q}' = \mathbb{R}'$ and $\mathbb{P}'(r) = r\mathbb{Q}'(r)$

$$\mathbb{P}(r) = \begin{cases} \mathbb{P}'(r) & \text{if } r > 1 \\ \dfrac{\mathbb{Q}'(r)}{\mathbb{Q}'(I)} \mathbb{P}'(I) & \text{if } r \in I \in \mathcal{I} \end{cases}$$

$\Rightarrow$

$\forall r \in I \in \mathcal{I}$
$$\frac{\mathbb{P}(r)}{\mathbb{Q}'(r)} = \frac{\mathbb{P}(I)}{\mathbb{Q}(I)}$$

$$\mathbb{Q}'(I) = \sum_{r \in I} \mathbb{Q}'(r)$$

All the ratios for $r \in I$ are the same
$\approx$ Merge

$\mathbb{R} \leftarrow$ **Sparsify_Left**$(\mathbb{R}')$ merge intervals $\mathcal{I} = \{[a_1, a_0), [a_2, a_1), \ldots, [a_m, a_{m-1})\}$

$\mathbb{R}' = (\mathbb{P}' || \mathbb{Q}')$, where $\mathbb{Q}' = \mathbb{R}'$ and $\mathbb{P}'(r) = r\mathbb{Q}'(r)$

$$\mathbb{P}(r) = \begin{cases} \mathbb{P}'(r) & \text{if } r > 1 \\ \dfrac{\mathbb{Q}'(r)}{\mathbb{Q}'(I)} \mathbb{P}'(I) & \text{if } r \in I \in \mathcal{I} \end{cases}$$

$$\mathbb{R} = (\mathbb{P} || \mathbb{Q}')$$

$$\Delta(\mathbb{R}', \mathbb{R}) \leq d_{TV}(\mathbb{P}', \mathbb{P}) + d_{TV}(\mathbb{Q}', \mathbb{Q}') = \frac{1}{2} \sum_{I \in \mathcal{I}} \sum_{r \in I} |\mathbb{P}'(r) - \mathbb{P}(r)|$$

$\mathbb{R} \leftarrow$ **Sparsify_Left**$(\mathbb{R}')$ merge intervals $L = \{[a_1, a_0), (a_2, a_1), \dots, (a_m, a_{m-1})\}$

$\mathbb{R}' = (\mathbb{P}'||\mathbb{Q}')$, where $\mathbb{Q}' = \mathbb{R}'$ and $\mathbb{P}'(r) = r\mathbb{Q}'(r)$

$$\mathbb{P}(r) = \begin{cases} \mathbb{P}'(r) & \text{if } r > 1 \\ \frac{\mathbb{Q}'(r)}{\mathbb{Q}'(I)}\mathbb{P}'(I) & \text{if } r \in I \in \mathcal{J} \end{cases}$$

$\Rightarrow$

$$\mathbb{R} = (\mathbb{P}||\mathbb{Q}')$$

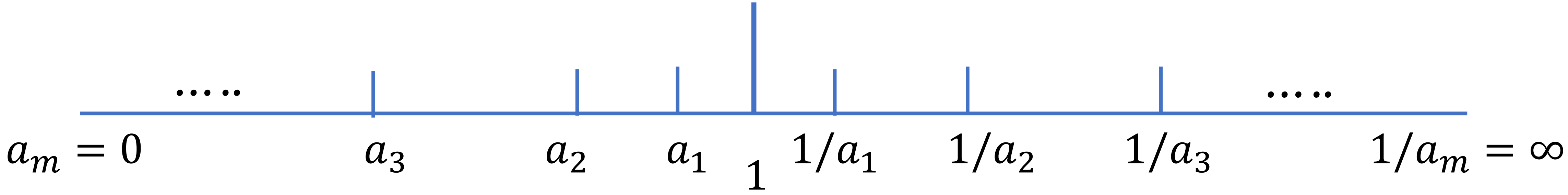
$$\Delta(\mathbb{R}', \mathbb{R}) \le \frac{1}{2}\sum_{I \in L}\sum_{r \in I}\mathbb{Q}'(r)\left|r - \frac{\mathbb{P}'(I)}{\mathbb{Q}'(I)}\right|$$

At most the length of interval $\le |a_i - a_{i-1}|$, where $I = [a_i, a_{i-1})$

vs

$$d_{TV}(\mathbb{R}') = \frac{1}{2}\sum_{I \in L \cup R}\sum_{r}\mathbb{Q}'(r)|r - 1|$$

At least the distance between 1 and right point $\ge 1 - a_{i-1}$



Partition of $[0,1]$

$[a_1, a_0 = 1)$
$[a_2, a_1)$
$[a_3, a_2)$
…
$[a_m, a_{m-1})$

Partition of $(1, \infty)$

$[a_0 = 1, 1/a_1)$
$[1/a_1, 1/a_2)$
$[1/a_2, 1/a_3)$
…
$[1/a_{m-1}, 1/a_m)$

- The first interval is small

$$1 - a_1 \leq \delta_s$$

- The length of $[a_i, a_{i-1}]$ is small w.r.t. $1 - a_{i-1}$

$$\forall i > 1, \qquad |a_i - a_{i-1}| \leq \epsilon_s \cdot |1 - a_{i-1}|$$

$$m = O\left(\frac{1}{\epsilon_s} \log \frac{1}{\delta_s}\right)$$

$\mathbb{R} \leftarrow$ **Sparsify_Left**$(\mathbb{R}')$ merge intervals $L = \{[a_1, a_0), (a_2, a_1), \dots, (a_m, a_{m-1})\}$

$$\mathbb{R}' = (\mathbb{P}' || \mathbb{Q}'), \text{ where } \mathbb{Q}' = \mathbb{R}' \text{ and } \mathbb{P}'(r) = r\mathbb{Q}'(r)$$

$$\mathbb{P}(r) = \begin{cases} \mathbb{P}'(r) & \text{if } r > 1 \\ \dfrac{\mathbb{Q}'(r)}{\mathbb{Q}'(I)} \mathbb{P}'(I) & \text{if } r \in I \in \mathcal{I} \end{cases}$$

$$\mathbb{R} = (\mathbb{P} || \mathbb{Q}')$$

$$\Delta(\mathbb{R}', \mathbb{R}) \leq \frac{1}{2}(\epsilon_s d_{TV}(\mathbb{R}') + \delta_s)$$

Error from merging other intervals

Error from merging the first interval