Distributional State Aggregation in Reinforcement Learning

August XX, 2020

Shayan Amani

Department of Computer Science, University of New Hampshire



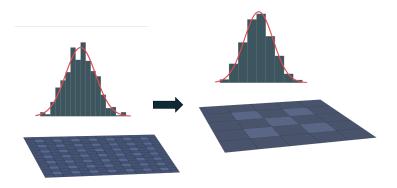
whoami



- ► Finished bachelor's in EE in spring 2015
- Aspired to develop for my own ideas
 - ▶ at a certain point, I had 200k monthly active users
- ▶ Started Ph.D. at UNH in fall 2017
- Have been experimenting with quite a few areas to discover what I like to pursue

Introduction

Problem



- ▶ Reduce model into low resolution clusters.
- ► Same distribution, different discritization in state space.

State Aggregation Problem

- ▶ No general rule applicable to various aggregation problems.
- ► Domain-dependent solutions.
- ▶ feature-based aggregation and more engineering.

Example





- ▶ 11 million taxi trips in Manhattan, NYC.
- ► Clustered into 1922 divisions.

Yaqi Duan, Zheng Tracy Ke, and Mengdi Wang. "State Aggregation Learning from Markov Transition Data". In: (2019), pp. 4486-4495. arXiv: 1811.02619. URL: http://papers.nips.cc/paper/8698-state-aggregation-learning-from-markov-transition-data.pdf.

State Aggregation Motivation

- less computational power
- ► more tractable problem
- analytically transparent approximation
 - ► compared to Neural Networks

State Aggregation Motivation

Steps toward an aggregation framework:

- ► Non-parametric
- ► Domain-agnostic
- Sample-based

Outline

- ► Introduction
- ► Density Estimation
- ▶ Histograms
- Metrics
- Methods
 - ► Environment
 - ► Interval Count
 - ► Interval Width
- Discussion
- ► Future Work
- ► Q&A

Density Estimation

Density Estimators

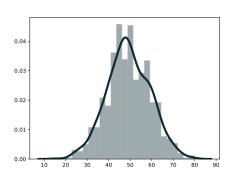
Definition:

Density estimation is fitting an estimate, based on **observed data** of an unobservable underlying **probability density function** (PDF).

Estimators:

- ▶ histogram
- kernel density estimation
- wavelets thresholding
- smoothing splines

Histogram Density Estimators



$$\hat{f}(x;w) = \frac{|B_j|}{nw}, \quad x \in B_j$$

Histograms

Pros Histogram

Advantages:

- As density estimators, histograms have been studied thoroughly for decades.
- ► Computational advantages compared to kernel-based methods.
- Non-parametric estimation to avoid domain-specific feature engineering.

Cons Histogram

Drawbacks:

- No universal optimality conditions on parameters (k, w) and asymptotic considerations.
- ► Cost of being non-parametric: slow convergence rate.
- Strong theoretical assumptions render theorems and results impractical.
- ► Computational complexity in case of non-normal distributions.

Goal Histogram

State aggregation based on histograms:

- Automatic and efficient method of choosing the number of bins.
- ▶ Based on the characteristics of the underlying distribution.

Metrics

Measure of Fit Histogram

- ▶ risk or integrated mean squared error (IMSE).
 - ▶ No direct solution to IMSE, underlying distribution is unknown
- estimated risk or cross-validation estimator of risk.

IMSE Measure of Fit

$$MSE{\hat{f}(.;w)} = \mathbb{E}\left[\hat{f}(x) - f(x)\right]^{2}$$

$$= \frac{1}{wk}\hat{f}(x) - \frac{1}{k}\hat{f}(x)^{2} + \left[\hat{f}(x) - f(x)\right]^{2}$$

$$= \frac{1}{wk}\hat{f}(x) - \frac{1}{k}\hat{f}(x)^{2} + \left[\hat{f}(x) - f(x)\right]^{2} \qquad (1)$$

$$= \frac{1}{wk}\hat{f}(x) - \frac{1}{k}\hat{f}(x)^{2} + \left[\hat{f}(x) - f(x)\right]^{2}$$

▶ The histogram converges in mean squared to f(x) if $w \to 0$ and $nw \to \infty$.

IMSE Measure of Fit

$$IMSE\{\hat{f}(.;w)\} = \int \mathbb{E}\{\hat{f}(x) - f(x)\}^2 dx$$
 (2)

- ► Global error measure of a histogram estimate.
- ▶ Slower convergence to a fixed-point than parametric estimators²: $n^{-2/3} > n^{-1}$

²Larry Wasserman. *All of Statistics; A Concise Course in Statistical Inference*. Springer Texts in Statistics. Springer New York, 2004. DOI: 10.1007/978-0-387-21736-9. URL:

Metrics How many bins?

Bias-Variance Tradeoff

Number of buckets of discritization:

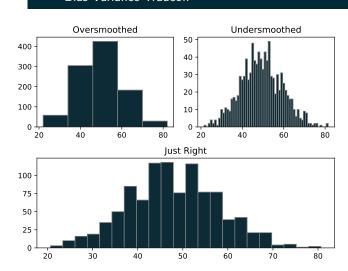
► range split aggregation

Variance Bias

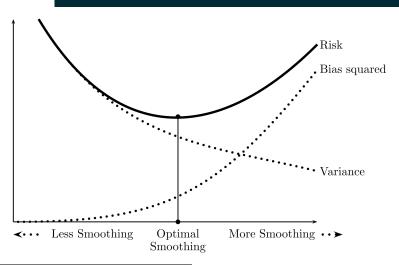
Bin-count Bin-width



Smoothing Bias-Variance Tradeoff



Optimal Smoothing Bias-Variance Tradeoff



Bin Count vs. Bin Width

For equally-spaced intervals:

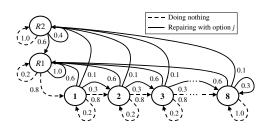
$$k = \left\lceil \frac{\max(x) - \min(x)}{w} \right\rceil \tag{3}$$

• depends on the distribution range and interval size: k = f(R, w)

Methods

Environment Method

Machine Replacement



Erick Delage and Shie Mannor. "Percentile optimization for Markov decision processes with parameter uncertainty". In: *Operations Research* 58.1 (2010), pp. 203–213. ISSN: 0030364X. DOI: 10.1287/opre.1080.0685.

Methods Interval Count Methods

Square-root Rule Interval Count

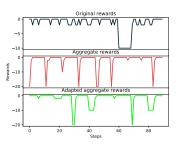
$$w = \frac{\max(x) - \min(x)}{\sqrt{n}} \tag{4}$$

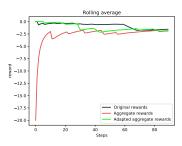
$$k = \lceil \sqrt{n} \rceil \tag{5}$$

- Intuitive: no restricting assumptions
- ► Used by Excel⁵.

⁵EXCEL Univariate: Histogram. URL:

Aggregation Square-root Rule





Sturge's Rule Interval Count

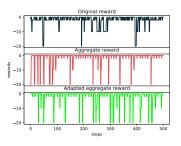
$$w = \frac{\max(x) - \min(x)}{1 + \lg n} \tag{6}$$

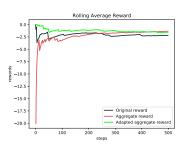
$$k = 1 + \lceil \lg n \rceil \tag{7}$$

- Estimates the original distribution with a series of binomial coefficients⁶.
- ▶ Normal distribution is implied.

⁶Herbert A. Sturges. "The Choice of a Class Interval". In: *Journal of the American Statistical Association* 21.153 (1926), pp. 65–66. URL: http://www.jstor.org/stable/2965501.

Aggregation Sturge's Formula





Rice Rule Interval Count

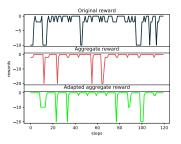
$$w = \frac{\max(x) - \min(x)}{2\sqrt[3]{n}} \tag{8}$$

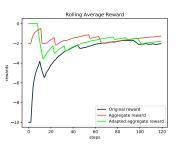
$$k = \lceil 2\sqrt[3]{n} \rceil \tag{9}$$

- ▶ The intuitive successor to Sturges' rule.
- Recommended by trial and errors⁷.

⁷David Lane. "Online Statistics Education: A Multimedia Course of Study".

Aggregation Rice Rule





Doane's Rule Interval Count

$$k = \underbrace{1 + \lceil \lg n \rceil}_{\text{Sturges' classes}} + \underbrace{\lceil \lg \left(1 + \frac{|\sqrt{\beta_1}|}{\sigma_{\sqrt{\beta_1}}}\right) \rceil}_{\text{Doane's extended classes}}$$

$$\sqrt{\beta_1} = \frac{m_3}{m_2^{3/2}} \tag{10}$$

$$m_2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2, m_3 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^3$$
 (11)

$$\sigma_{\sqrt{\beta_1}} = \sqrt{\frac{6(n-2)}{(n+1)(n+3)}} \tag{12}$$

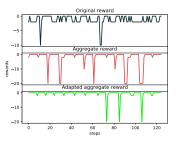
Doane's Formula Interval Count

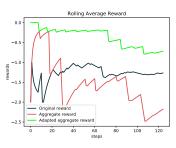
- Modified Sturges' formula to reflect distribution characteristics⁸.
- ► Hence, performs better in case of skewed distributions⁹.
- ▶ Inspired by coding in the information theory: increasing entropy by introducing more symbols for coding.

⁸David P Doane. *Aesthetic Frequency Classifications*. Tech. rep. 4. 1976, pp. 181–183.

⁹David P Doane and Lori E Seward. *Measuring Skewness: A Forgotten Statistic?*. Tech. rep. 2. 2011. URL: www.amstat.org/publications/jse/v19n2/doane.pdf.

Aggregation Doane's Formula





Methods Interval Width Methods

Scott's Formula Interval Width

$$IMSE = \int E\{\hat{f}(x) - f(x)\}^2 dx$$
 (13)

using Taylor expansion:

IMSE =
$$1/(nw) + \frac{1}{12}w^2 \int_{-\infty}^{\infty} f'(x)^2 dx + O(1/n + w^3)$$
 (14)

$$w^* = \left\{ 6 \middle/ \int_{-\infty}^{\infty} f'(x)^2 dx \right\}^{1/3} n^{-1/3}$$
 (15)

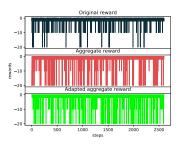
$$w^* = 2\sqrt[6]{9\pi} \sigma n^{-1/3}$$

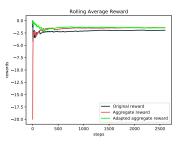
= 3.49083 \sigma n^{-1/3} (16)

Scott's Formula Interval Width

- ▶ Calculates the w^* by minimizing IMSE¹⁰.
- ▶ Derived the estimate for a Gaussian distribution.

Aggregation Scott's Formula



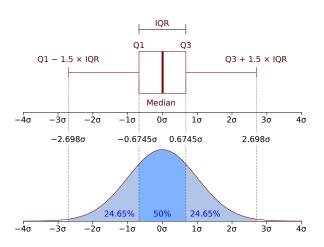


Freedman-Diaconis' Rule Interval Width

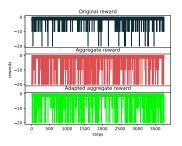
$$w = 2 \, \text{IQR}(x) \, n^{-1/3}$$
 (17)

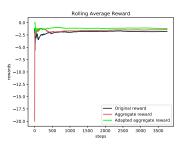
- ▶ $3.5 \sigma \approx 2 IQR$
- ▶ More robustness to outliers than standard deviation

IQR <u>Free</u>dman-Diaconis' Rule



Aggregation Freedman-Diaconis' Rule





Shimazaki-Shinomoto's Choice Interval Width

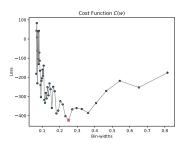
$$w^* = \underset{w}{\operatorname{arg\,min}} C(w) = \underset{w}{\operatorname{arg\,min}} \frac{2\bar{X} - \sigma^2}{w^2}$$

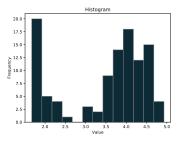
$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i; \ \underline{\sigma^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X})^2}$$
biased variance

- ► Minimizes cost function for a set of proposed bin-widths¹².
- ► Looks over the dispersion of data points count falling into bins.

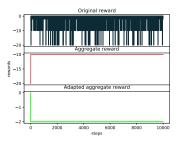
¹²Hideaki Shimazaki and Shigeru Shinomoto. "A recipe for optimizing a time-histogram". In: *Advances in Neural Information Processing Systems*. 2007, pp. 1289–1296. ISBN: 9780262195683.

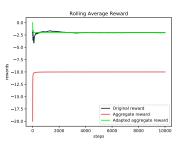
Cost Analysis Shimazaki-Shinomoto's Choice





Aggregation Shimazaki-Shinomoto's Choice





Discussion

- Incorporating more characteristics of underlying distribution leads to a better aggregation policy.
- ► High dimensional spaces may take more advantage of this approach.
- Sampling distribution decently explains the candidacy of states for aggregation.

Ideas for Future

- 1. Adjusted Fisher-Pearson estimation of skewness to take sample size into account.
- Employ studentized test instead of kurtosis in Doane's formula¹³,¹⁴.
- 3. Variable bin-width aggregation.

¹³R C Geary. Moments of the Ratio of the Mean Deviation to the Standard Deviation for Normal Samples. Tech. rep. 3. 1936, pp. 295–307.

¹⁴Ronald L. Tracy and David P. Doane. "Using The Studentized Range to Assess Kurtosis". In: *Journal of Applied Statistics* 32.3 (2005), pp. 271–280. ISSN: 02664763. DOI: 10.1080/02664760500054632.

Questions

They have said...

"Our virtues and our failings are **inseparable**, like force and matter. **When they**separate, man is no more."

Nikola Tesla

- Duan, Yaqi, Zheng Tracy Ke, and Mengdi Wang. "State
 Aggregation Learning from Markov Transition Data". In:
 (2019), pp. 4486-4495. arXiv: 1811.02619. URL:
 http://papers.nips.cc/paper/8698-state-aggregation-learning-from-markov-transition-data.pdf.
- Wasserman, Larry. All of Statistics; A Concise Course in Statistical Inference. Springer Texts in Statistics. Springer New York, 2004. DOI: 10.1007/978-0-387-21736-9. URL: http://link.springer.com/10.1007/978-0-387-21736-9.
- Delage, Erick and Shie Mannor. "Percentile optimization for Markov decision processes with parameter uncertainty". In: Operations Research 58.1 (2010), pp. 203–213. ISSN: 0030364X. DOI: 10.1287/opre.1080.0685.
- EXCEL Univariate: Histogram. URL: http: //cameron.econ.ucdavis.edu/excel/ex11histogram.html.
 - Sturges, Herbert A. "The Choice of a Class Interval". In: Journal of the American Statistical Association 21.153 (1926), pp. 65-66. URL: http://www.jstor.org/stable/2965501.

- Lane, David. "Online Statistics Education: A Multimedia Course of Study". In: EdMedia + Innovate Learning 2003.1 (2003), pp. 1317–1320.
- Doane, David P. Aesthetic Frequency Classifications. Tech. rep. 4. 1976, pp. 181–183.
- Doane, David P and Lori E Seward. Measuring Skewness: A
 Forgotten Statistic?. Tech. rep. 2. 2011. URL:
 www.amstat.org/publications/jse/v19n2/doane.pdf.
 Scott, David W. "On optimal and data-based histograms". In
- Scott, David W. "On optimal and data-based histograms". In: Source: Biometrika 66.3 (1979), pp. 605–610.
- Shimazaki, Hideaki and Shigeru Shinomoto. "A recipe for optimizing a time-histogram". In: Advances in Neural Information Processing Systems. 2007, pp. 1289–1296. ISBN: 9780262195683.
- Geary, R C. Moments of the Ratio of the Mean Deviation to the Standard Deviation for Normal Samples. Tech. rep. 3. 1936, pp. 295–307.

Tracy, Ronald L. and David P. Doane. "Using The Studentized Range to Assess Kurtosis". In: *Journal of Applied Statistics* 32.3 (2005), pp. 271–280. ISSN: 02664763. DOI: 10.1080/02664760500054632.