WORK DISTRIBUTION IS REALISED FOR OVERDAMPED LANGEVEN EQUATION WITH HOLONOMIC CONSTRAINTS

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November 9, 2024

ABSTRACT

Jarzynski equality is the relation between work and free energy differece. To calculate the free energy, we need to compute exponential average of the work, and this is really painful. To stay out of the exponential average, we often use the second order cumunant expansion. This is exact if work distribution is Gaussian. However, the assumption is not always the case. It proved to be true if a harmonically steered dynamics obeys overdamped Langevin equation [Shulten et al.]. Here, I prove the work distribution to be Gaussian under the assumption that overdamped Langevin equation with holonomic constraints. This result benefits the application of free energy estimation via targeted molecular dynamics, in particular.

1 Introduction

Our project is a competition on Kaggle (Predict Future Sales). We are provided with daily historical sales data (including each products' sale date, block ,shop price and amount). And we will use it to forecast the total amount of each product sold next month. Because of the list of shops and products slightly changes every month. We need to create a robust model that can handle such situations.

$$\Delta G = -\beta^{-1} \ln \left[\langle e^{-\beta W} \rangle \right] \tag{1}$$

2 Theory

Result 1. *Cumulant expansion*

Task modeling. We approach this task as a regression problem. For every item and shop pair, we need to predict its next month sales(a number).

Construct train and test data. In the Sales train dataset, it only provides the sale within one day, but we need to predict the sale of next month. So we sum the day's sale into month's sale group by item, shop, date(within a month). In the Sales train dataset, it only contains two columns(item id and shop id). Because we need to provide the sales of next month, we add a date column for it, which stand for the date information of next month.

2.1 Headings: second level

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$$\xi_{ij}(t) = P(x_t = i, x_{t+1} = j | y, v, w; \theta) = \frac{\alpha_i(t) a^{w_t}_{ij} \beta_j(t+1) b^{v_{t+1}}_j (y_{t+1})}{\sum^N_{i=1} \sum^N_{j=1} \alpha_i(t) a^{w_t}_{ij} \beta_j(t+1) b^{v_{t+1}}_j (y_{t+1})} \tag{2}$$

2.1.1 Headings: third level

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3 Examples of citations, figures, tables, references

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The documentation for `natbib` may be found at

`http://mirrors.ctan.org/macros/latex/contrib/natbib/natnotes.pdf`

Of note is the command `\citet`, which produces citations appropriate for use in inline text. For example,

```
\citet{hasselmo} investigated\dots
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produces

> Hasselmo, et al. (1995) investigated…

`https://www.ctan.org/pkg/booktabs`

3.1 Figures

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[1] Sample of the first footnote.

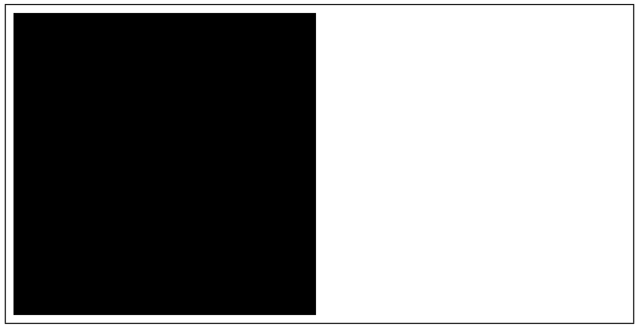

Figure 1: Sample figure caption.

Table 1: Sample table title

Part		
Name	Description	Size (μm)
Dendrite	Input terminal	$\sim$100
Axon	Output terminal	$\sim$10
Soma	Cell body	up to 10^6

3.2 Tables

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3.3 Lists

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- consectetur adipiscing elit.
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References

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