## Deduce: Deviation of mutual information estimation

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$$I_{true}(X;Y) = \int_{y} \int_{x} F(x,y) log \frac{F(x,y)}{f(x)g(y)} dxdy$$

$$= \sum_{y_{i}} \sum_{x_{i}} \int_{y_{i}}^{y_{i}+\triangle y} \int_{x_{i}}^{x_{i}+\triangle x} F(x,y) log \frac{F(x,y)}{f(x)g(y)} dxdy$$

$$= \sum_{y_{i}} \sum_{x_{i}} F(x_{i}^{c}, y_{i}^{c}) log \frac{F(x_{i}^{c}, y_{i}^{c})}{f(x_{i}^{c})g(y_{i}^{c})} \triangle x \triangle y$$

$$(0.1)$$

$$I_{obs}(X;Y) = \sum_{y} \sum_{x} P(x,y) log \frac{P(x,y)}{P(x)P(y)}$$

$$(0.2)$$

$$P(x_i, y_j) = \int_{\triangle y} \int_{\triangle x} F(x_i, y_j) dx_i dy_j = F(\hat{x}_i, \hat{y}_j) \triangle x \triangle y$$
(0.3)

Similarly,

$$P(x_i) = f(\tilde{x}_i) \triangle x$$

$$P(y_i) = g(\tilde{y}_i) \triangle y$$
(0.4)

Here, take Taylor expension of  $F(x_i^c, y_j^c)$ ,  $f(x_i^c)$ ,  $g(y_j^c)$  around  $(x,y) = (\hat{x}_i, \hat{y}_j)$ ,  $x = \tilde{x}_i$ ,  $y = \tilde{y}_j$ , respectively.

$$F(x_{i}^{c}, y_{j}^{c}) = F(\hat{x}_{i}, \hat{y}_{j}) + \frac{\partial F}{\partial x}(x_{i}^{c} - \hat{x}_{i}) + \frac{\partial F}{\partial y}(y_{j}^{c} - \hat{y}_{j}) + \frac{1}{2} \frac{\partial^{2} F}{\partial x \partial y}(x_{i}^{c} - \hat{x}_{i})(y_{j}^{c} - \hat{y}_{j}) + \dots$$

$$f(x_{i}^{c}) = f(\tilde{x}_{i}) + \frac{df}{dx}(x_{i}^{c} - \tilde{x}_{i}) + \frac{1}{2} \frac{d^{2} f}{dy}(x_{i}^{c} - \tilde{x}_{i})^{2} + \dots$$

$$g(y_{j}^{c}) = g(\tilde{y}_{j}) + \frac{dg}{dy}(y_{j}^{c} - \tilde{y}_{j}) + \frac{1}{2} \frac{d^{2} g}{dy}(y_{j}^{c} - \tilde{y}_{j})^{2} + \dots$$

$$(0.5)$$

Since  $|x_i^c - \hat{x}_i| \le \Delta x$ ,  $|y_j^c - \hat{y}_j| \le \Delta y$ ,  $\Delta x = \Delta y = h$ ,

$$F(x_i^c, y_j^c) = F(\hat{x}_i, \hat{y}_j) + \left(\frac{\partial F}{\partial x}\hat{c}_i + \frac{\partial F}{\partial y}\hat{c}_j\right)h + O(h^2)$$

$$f(x_i^c) = f(\tilde{x}_i) + \frac{df}{dx}\tilde{c}_ih + O(h^2)$$

$$g(y_j^c) = g(\tilde{y}_j) + \frac{dg}{dy}\tilde{c}_jh + O(h^2)$$

$$(0.6)$$

Substitute those expression into the expression of mutual information.

$$I_{true}(X;Y) \doteq \sum_{y_i} \sum_{x_i} F(x_i^c, y_i^c) \triangle x \triangle y [log(F(x_i^c, y_i^c) \triangle x \triangle y) - log(f(x_i^c) \triangle x) - log(g(y_i^c) \triangle y)]$$

$$= \sum_{y_i} \sum_{x_i} [P(x_i, y_j) + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3]$$

$$[log(P(x_i, y_j) + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3) - log(P(x_i) + \frac{df}{dx} \tilde{c}_i h^2) - log(P(y_j) + \frac{dg}{dy} \tilde{c}_j h^2))]$$

$$(0.7)$$

Take Taylor expansion of logarithmic function to the first order,

$$I_{true}(X;Y) \doteq \sum_{y_i} \sum_{x_i} (P(x_i, y_j) + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3)$$

$$(log P(x_i, y_j) + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3 - log P(x_i) - \frac{df}{dx} \tilde{c}_i h^2 - log P(y_j) - \frac{dg}{dy} \tilde{c}_j h^2)$$

$$= \sum_{y_i} \sum_{x_i} (P(x_i, y_j) + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3)$$

$$(log \frac{P(x_i, y_j)}{P(x_i) P(y_j)} + (\frac{\partial F}{\partial x} \hat{c}_i + \frac{\partial F}{\partial y} \hat{c}_j) h^3 - (\frac{df}{dx} \tilde{c}_i + \frac{dg}{dy} \tilde{c}_j) h^2)$$

$$(0.8)$$

Drop higher order terms which is sufficiently smaller than  $O(h^2)$ .

$$I_{true}(X;Y) \doteq \sum_{y_j} \sum_{x_i} P(x_i, y_j) (log P(x_i, y_j) - log P(x_i) - \frac{df}{dx} \tilde{c}_i h^2 - log P(y_j) - \frac{dg}{dy} \tilde{c}_j h^2)$$

$$= \sum_{y_j} \sum_{x_i} P(x_i, y_j) (log \frac{P(x_i, y_j)}{P(x_i) P(y_j)} - (\frac{df}{dx} \tilde{c}_i + \frac{dg}{dy} \tilde{c}_j) h^2)$$

$$= I_{obs} - \sum_{y_i} \sum_{x_i} P(x_i, y_j) (\frac{df}{dx} \tilde{c}_i + \frac{dg}{dy} \tilde{c}_j) h^2$$

$$(0.9)$$

Since  $\tilde{c}_i$  and  $\tilde{c}_j$  are constants, they can obsorbe the negative sign outside the summation. Therefore, the deviation of mutual information estimation with finite, equally binned histogram from its true value given by the expression below:

$$I_{true} - I_{obs} = h^2 \sum_{y_i} \sum_{x_i} P(x_i, y_j) \left(\frac{df}{dx} \tilde{c}_i + \frac{dg}{dy} \tilde{c}_j\right) + O(h^3)$$
(0.10)

In the next part, numerical results are presented to varify the analytical results above. X and Y are two random variables generated by the following equations.

$$\begin{cases} X = \epsilon \\ Y = \beta \eta_1 + \xi X + \eta_2 \end{cases}$$

where  $\epsilon$  and  $\eta_i$  are independent normally distributed random variables, and  $\beta$  and  $\xi$  are interacting strength between variables. Here, X and Y both contain  $10^8$  independent samples. We calculate the mutual information between X and Y using theoretical expression and numerical estimation, respectively. And we can get the deviation of mutual information estimation from its true value, which given by theoretical expression, as a function of binning size.

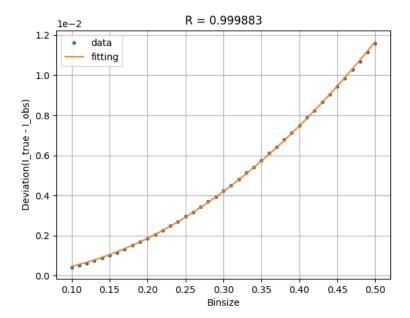


Figure 0.1: Accuracy of mutual information estimation as a function of bin size of histograms of variables.

We find that the data points are nicely fitted by second order polynomial given by  $y = ax^2$ . This result verify our deduction above.

Then we move the case for mutual information between binary spike train X and continues neuronal data Y, which is net synaptic current of single neuron. We demonstrate a two excitatory neuron system simulated with conductance-based leaky integrate-and-fire model. Two neuron, which labeled as neuron-1 and neuron-2 respectively, are one-way connected, meaning neuron-1 can transmit its spike train to neuron-2 but not counterwise. We record spike train from neuron-1 as X and synaptic current from neuron-2 as Y. The simulating parameters of this system are listed below.

Total time period	$10^8 \text{ ms}$
Recording rate	$2\ ms^-1$
Synaptic strength	$5^{-}2$
Poisson rate	$1.3~\mathrm{kHz}$
Poisson strength	$5^{-2}$

Since X is a binary variable, the expression in 0.10 needs to be modified.

$$I_{true} - I_{obs} = h^2 \left[ \sum_{y_i} \frac{\partial F}{\partial y} \bigg|_{x=0} c_i log \frac{P(x=0, y_i)}{P(x=0)P(y_i)} + \frac{\partial F}{\partial y} \bigg|_{x=1} c_i' log \frac{P(x=1, y_i)}{P(x=1)P(y_i)} + P(x=0, y_i) \left( \frac{\partial F}{\partial y} \bigg|_{x=0} c_i - \frac{dg}{dy} \hat{c}_i + P(x=1, y_i) \left( \frac{\partial F}{\partial y} \bigg|_{x=1} c_i' \right) - \frac{dg}{dy} \hat{c}_i' \right) \right] + o(h^2)$$

$$(0.11)$$

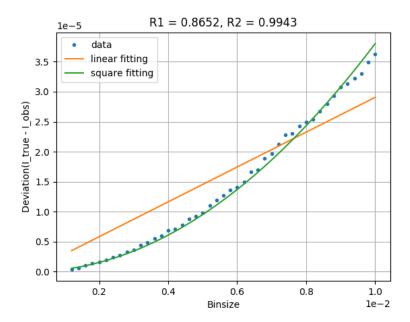


Figure 0.2: Accuracy of mutual information estimation as a function of bin size of histograms of variables.

The orange line is the linear fitting given by y = ax and the green curve is the square fitting given by  $y = ax^2$ .