Entropy and information of undersampled probability distributions

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http://arxiv.org/abs/physics/0306063
http://arxiv.org/abs/physics/0207009
http://arxiv.org/abs/physics/0108025
http://arxiv.org/abs/physics/0103088
Talk outline

Problem setup  Estimation information contents of spike trains, genomic sequences.
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Developing intuition  Why is it so difficult to estimate entropies?
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The method  An idea.
The method  Analysis.
The method  Asymptotics.
The method  Synthetic experiments.
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The method  An idea.

The method  Analysis.

The method  Asymptotics.

The method  Synthetic experiments.

Applications  Dealing with undersampling in neural data.

Applications  Hints at future results.
Neurophysiological recordings

Strong et al., 1998
Neurophysiological recordings

Strong et al., 1998

Neurons communicate by stereotypical pulses (spikes). Information is transmitted by spike rates and (possibly) precise positions of the spikes.
Estimating information rate in spike trains

\[ T=4 \]

\[ N=5 \]

\[ P(W) \rightarrow S(W) = S^t \]

\[ I = S^t - S^n \]
Experimental setup

Lewen, Bialek, and de Ruyter

van Steveninck, 2001
Experimental setup

Lewan, Bialek, and de Ruyter van Steveninck, 2001

Bialek and de Ruyter van Steveninck, 2002, Land and Collett 1974
Recordings and problems

100–200 repeats of 5–10 s roller coasters rides
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4. Need to have $\Delta \approx 100\text{ms}$ due to natural stimulus correlations.
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Need to estimate entropies of words of length $\sim 40$ from $< 200$ samples.
Genomics analysis

\[ \text{GCCTA}\overbrace{\text{ACCGT}}^{N} \overbrace{\text{GGTCCA}}^{M} \underbrace{\text{TATATATA}}_{D} \text{AGGAA} \]
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Estimate mutual information \( I(M, N; D) \).
Genomics analysis

Estimate mutual information $I(M, N; D)$. Study predictability properties.
Genomics analysis

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Study predictability properties.

Search for motifs.
Genomics analysis

Estimate mutual information $I(M, N; D)$.
Study predictability properties.
Search for motifs.
Run IB and extract predictive features.
Why is it difficult to estimate entropies?

Suppose $\epsilon$ of the probability mass is in $K$ (unknown) number of bins.
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$$\{Q_1, Q_2\} \longrightarrow \{n_1, n_2\}$$

$$\longrightarrow \{Q_1 + \delta, Q_2 - \delta\} \longrightarrow S - S_{\text{true}} < 0$$

Last step due to nonlinearity of $\log_2 P$. 
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Undersampling: metric cases
(weather, stocks,...)

Possible outcomes
Probability density
Observed data
Undersampled regime
Smoothness
Regularization of learning
Model selection
Prior-insensitive learning

\[ x, a \leq x \leq b \]
\[ Q(x) \]
\[ x_{\mu}, \mu = 1 \ldots N \]
always

\[ \frac{\partial^n Q}{\partial x^n} \text{ is small} \]
local: punish for \( \frac{\partial^n Q}{\partial x^n} \gg 1 \)
phase space volume, self-consistent
probably possible
Undersampling: non–metric cases
(languages, bioinformatics,...)

Discrete outcomes (bins) \( i, i = 1 \ldots K \)
Probability mass \( q_i \)
Observed bin occupancy \( n_i \)
Undersampled regime \( \sum_{i=1}^{K} n_i \equiv N \ll K \)
Smoothness undefined
Regularization of learning ultralocal: \( \mathcal{P}(\{q_i\}) = \prod \mathcal{P}_i(q_i) \)
global: \( \mathcal{P}(\{q_i\}) = F(\text{entropy}) \)
Model selection unknown
Prior-insensitive learning probably impossible for \( N \ll K \)
We choose . . .

(for discrete case)
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(for discrete case)

1. Define smoothness as high entropy or low mutual information distributions.
We choose . . .

(for discrete case)

1. Define smoothness as high entropy or low mutual information distributions.

2. Prior-insensitive learning of useful functionals (like entropy) may be possible for $N \ll K$ even if it’s impossible for $\{q_i\}$ (these are just a few numbers).
Learning with nearly uniform priors
(ultra–local, Dirichlet priors)

\[ \mathcal{P}_\beta(\{q_i\}) = \frac{1}{Z(\beta)} \delta \left( 1 - \sum_{i=1}^{K} q_i \right) \prod_{i=1}^{K} q_i^{\beta - 1} \]
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Some common choices:
Maximum likelihood \[ \beta \rightarrow 0 \]
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- Laplace’s successor rule  \( \beta = 1 \)
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- Maximum likelihood: \( \beta \to 0 \)
- Laplace’s successor rule: \( \beta = 1 \)
- Krichevsky–Trofimov (Jeffreys) estimator: \( \beta = 1/2 \)
- Schurmann–Grassberger estimator: \( \beta = 1/K \)
Numerics of the Dirichlet family

To generate distributions: Successively select each $q_i$ according to

$$P(q_i) = B \left( \frac{q_i}{1 - \sum_{j<i} q_j}; \beta, (K - i)\beta \right)$$

$$B(x; a, b) = \frac{x^{a-1}(1-x)^{b-1}}{B(a, b)}$$
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Typical distributions ($K = 1000$). Note that the $\beta = 1$ distribution is very non-uniform, but has almost the maximum entropy (maybe reorder bins?)

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Bayesian inference with Dirichlet priors

\[ P_\beta(\{q_i\}|\{n_i\}) = \frac{P(\{n_i\}|\{q_i\})P_\beta(\{q_i\})}{P_\beta(\{n_i\})} \]

\[ P(\{n_i\}|\{q_i\}) = \frac{K}{\prod_{i=1}^{K} (q_i)^{n_i}} \]

\[ \langle q_i \rangle_\beta = \frac{n_i + \beta}{N + K\beta} \]
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Equal pseudocounts added to each bin.
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Equal pseudocounts added to each bin.

Larger $\beta$ means less sensitivity to data, thus more smoothing.
A problem: A priori entropy expectation

\[ P_\beta(S) = \int dq_1 dq_2 \cdots dq_K P_\beta(\{q_i\}) \delta \left[ S + \sum_{i=1}^{K} q_i \log_2 q_i \right] \]
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\[ \mathcal{P}_\beta(S) = \int dq_1 dq_2 \cdots dq_K P_\beta(q_i) \delta \left[ S + \sum_{i=1}^{K} q_i \log_2 q_i \right] \]

\[ \xi(\beta) \equiv \langle S[n_i = 0] \rangle_\beta \]

\[ = \psi_0(K\beta + 1) - \psi_0(\beta + 1) , \]

\[ \sigma^2(\beta) \equiv \langle (\delta S)^2[n_i = 0] \rangle_\beta \]

\[ = \frac{\beta + 1}{K\beta + 1} \psi_1(\beta + 1) - \psi_1(K\beta + 1) \]

\[ \psi_m(x) = (d/dx)^{m+1} \log_2 \Gamma(x) \text{ –the polygamma function} \]
The problem: Analysis
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2. Narrow peak: \( \max \sigma(\beta) = 0.61 \text{ bits} \ll \log_2 K \) at \( \beta \approx 1/K \); \( \sigma(\beta) \propto 1/\sqrt{K\beta} \) for \( K\beta \gg 1 \); \( \sigma(\beta) \propto \sqrt{K\beta} \) for \( K\beta \ll 1 \).
The problem: Analysis

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3. As \( \beta \) varies from 0 to \( \infty \), the peak smoothly moves from \( \xi(\beta) = 0 \) to \( \log_2 K \). For any finite \( \beta \), \( \xi(\beta) = \log_2 K - O(K^0) \).
The problem

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4. All common estimators are, therefore, bad for learning entropies.
Problems of common estimators

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\[ \sigma(1/K) \approx 0.61 \text{ bit} \]

(least biased)

Schurmann–Grassberger
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**Laplace and KT**

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**Schurmann–Grassberger**

Still strongly biased towards
\[ S = 1/\ln 2 \text{ bits.} \]
Removing the entropy bias at the source

Need such $\mathcal{P}(\{q_i\})$ that $\mathcal{P}(S[q_i])$ is (almost) uniform.
Removing the entropy bias at the source

Need such $\mathcal{P}(\{q_i\})$ that $\mathcal{P}(S[q_i])$ is (almost) uniform.

Our options:

1. $\mathcal{P}_{\beta}^{\text{flat}}(\{q_i\}) = \frac{\mathcal{P}_\beta(\{q_i\})}{\mathcal{P}_\beta(S[q_i])}$. 
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2. $\mathcal{P}(S) \sim 1 = \int \delta(S - \xi) d\xi$. Easy: $\mathcal{P}_\beta(S)$ is almost a $\delta$-function!
Solution

Average over $\beta$ — infinite Dirichlet mixtures.

\[
\mathcal{P}(\{q_i\}; \beta) = \frac{1}{\mathcal{Z}} \delta \left( 1 - \sum_{i=1}^{K} q_i \right) \prod_{i=1}^{K} q_i^{\beta-1} \frac{d\xi(\beta)}{d\beta} \mathcal{P}(\xi(\beta))
\]

\[
\hat{S}_m = \int d\xi \rho(\xi, \{n_i\}) \langle S_m[n_i] \rangle_{\beta(\xi)} \frac{\Gamma(K\beta(\xi))}{\Gamma(N + K\beta(\xi))} \prod_{i=1}^{K} \frac{\Gamma(n_i + \beta(\xi))}{\Gamma(\beta(\xi))}.
\]
1. $d\xi/d\beta$ insures a priori uniformity over expected entropy.
Solution: explanations

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2. \(P(\xi)\) embodies actual expectations about entropy.
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4. If \( \rho(\xi) \) is peaked, then some \( \beta(\xi) \) (model) dominates (is “selected”), and the variance of the estimator is small.
Too rough or too smooth?

Typical rank–ordered plots:

\[ q_i \approx 1 - \left[ \frac{\beta B(\beta, \kappa - \beta)(K - 1)i}{K} \right]^{1/(\kappa - \beta)}, \quad i \ll K, \]

\[ q_i \approx \left[ \frac{\beta B(\beta, \kappa - \beta)(K - i + 1)}{K} \right]^{1/\beta}, \quad K - i + 1 \ll K \]
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Usually only the first regime is observed.
First attempts to estimate entropy

Typical distributions

\[ \beta = 0.0007 \quad S = 1.05 \text{ bits} \]

\[ \beta = 0.02 \quad S = 5.16 \text{ bits} \]

\[ \beta = 1.0 \quad S = 9.35 \text{ bits} \]
First attempts to estimate entropy

Typical distributions

Atypical distributions

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Estimating entropy: first observations

1. Relative error $\sim 10\%$ at $N$ as low as 30 for $K = 1000$. 
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Estimating entropy: first observations

1. Relative error $\sim 10\%$ at $N$ as low as 30 for $K = 1000$.
2. Reliable estimation of error (posterior variance).
3. *Little bias*, as it should be. Exception: too smooth distributions.
4. **Key point**: *learn entropies directly without finding* $\{q_i\}$!
5. The dominant $\beta$ stabilizes for typical distributions; drifts down (to complex models) for rough ones and up (to simpler models) for too smooth cases.
Asymptotics – many coincidences

For $K \gg N \gg 1$, and $\Delta \equiv N - K$ (nonzero counts) $\equiv N\delta \gg 1$, find 

$$\beta^* = \kappa^* / N$$ (saddle point).

$$\kappa^* = \kappa_0 + \frac{1}{K}\kappa_1 + \frac{1}{K^2}\kappa_2 + \ldots$$
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other $\kappa_i$ and $b_i$ are $O(1)$
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\kappa_0 = N\left(\frac{b^{-1}}{\delta} + b_0 + b_1\delta + \ldots\right)
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\[
\left.\frac{\partial^2 (-\log \rho)}{\partial \xi^2}\right|_{\xi(\beta^*)} = \left[\frac{\partial^2 (-\log \rho)}{\partial \beta^2} \frac{1}{(d\xi/d\beta)^2}\right]_{\beta^*} = \Delta + NO(\delta^2)
\]
Asymptotics – few coincidences

For $K \to \infty$, $\Delta \sim 1$, $\delta \to 0$

$$\hat{S} \approx (C_\gamma - \ln 2) + 2 \ln N - \psi_0(\Delta) + O\left(\frac{1}{N}, \frac{1}{K}\right)$$

$$\left(\delta S\right)^2 \approx \psi_1(\Delta) + O\left(\frac{1}{N}, \frac{1}{K}\right)$$
Estimator: Properties

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6. The estimator should work (in some cases) for $N \ll K$, $N \ll 2^S$, and $N \sim 2^{S/2}$ (cf. Ma, 1981).
Estimator: Synthetic test

Refractory Poisson process: \( r = 0.26 \text{ms}^{-1}, \ R = 1.8 \text{ms}, \ T = 15 \text{ms}, \ \tau = 0.5 \text{ms}. \)
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Estimator is unbiased if it is consistent and agrees with itself for all $N$ within error bars.
Natural data: Slice entropy vs. sample size

Slice at 1800 ms, $\tau = 2$ ms, $T = 16$ ms

$Ilya Nemenman, CompBio seminar, Columbia U, February 13, 2004$
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$S_n(T,\tau)$, bits

ML estimator converges with $\sim 1/N$ corrections.
Natural data: Slice entropy vs. sample size

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$1/N$

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$\frac{S_{\text{NSB}} - S_{\text{ML}}}{\delta S_{\text{NSB}}}$ has zero mean if $S_{\text{ML}}$ is reliable.

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Natural data: Error vs. mean

\[ \epsilon(N) \equiv \frac{S_{NSB}(N) - S}{\delta S_{NSB}(N)} \approx \frac{S_{NSB}(N) - S_{NSB}(196)}{\delta S_{NSB}(N)}. \]

Remember: \( \log_2 196 \approx 7.5 \text{bit}. \)
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Almost no bias.

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Empirical variance < 1 due to long tails in posterior.
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Almost no bias. 
Empirical variance $< 1$ due to long tails in posterior. 
Bands are due to discrete nature of $\Delta$.

Ilya Nemenman, CompBio seminar, Columbia U, February 13, 2004
Natural data: Hints of future results

Some preliminary results for information rate estimation. Further work is needed to properly estimate error bars due to signal correlations.
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Conclusions

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3. Neural data seems to be well matched to the estimator.