Zipf’s law and criticality in multivariate data without fine-tuning

David J. Schwab†

Department of Physics and Lewis-Sigler Institute, Princeton University, Princeton, NJ 08854

Ilya Nemenman†

Departments of Physics and Biology, Emory University, Atlanta, GA 30322

Pankaj Mehta‡

Department of Physics, Boston University, Boston, MA 02215

The joint probability distribution of many degrees of freedom in biological systems, such as firing patterns in neural networks or antibody sequence composition in zebrafish, often follow Zipf’s law, where a power law is observed on a rank-frequency plot. This behavior has recently been shown to imply that these systems reside near to a unique critical point where the extensive parts of the entropy and energy are exactly equal. Here we show analytically, and via numerical simulations, that Zipf-like probability distributions arise naturally if there is an unobserved variable (or variables) that affects the system, e. g. for neural networks an input stimulus that causes individual neurons in the network to fire at time-varying rates. In statistics and machine learning, these models are called latent-variable or mixture models. Our model shows that no fine-tuning is required, i.e. Zipf’s law arises generically without tuning parameters to a point, and gives insight into the ubiquity of Zipf’s law in a wide range of systems.

Advances in high throughput experimental biology now allow the joint measurement of activities of many basic components underlying collective behaviors in biological systems. These include firing patterns of many neurons responding to a movie [13], sequences of proteins from individual immune cells in zebrafish [5,6], protein sequences more generally [7,8], and even the simultaneous motion of flocking birds [9]. A remarkable result of these data and their models has been the observation that these large biological systems often reside close to a critical point [10]. This is most clearly manifest directly from the data by the following striking behavior. If we order the states, $\sigma$, of a system by decreasing probability, then the frequency of the states decays as the inverse of their rank, $r(\sigma)$, to some power:

$$P(\sigma) \propto \frac{1}{r(\sigma)^\alpha}. \quad (1)$$

Many systems in fact exhibit $\alpha \simeq 1$, which is termed Zipf’s law, and on which we will focus.

It has been argued that Zipf’s law is a model-free signature of criticality in the underlying system, using the language of statistical mechanics [10]. Without loss of generality, we can define the “energy” of a state $\sigma$ to be

$$E(\sigma) = -\log P(\sigma) + \text{const.} \quad (2)$$

The additive constant is arbitrary, and the temperature is $k_B T = 1$. We can also define the “entropy”, $S(E)$, using the density of states, $\rho(E) = \sum_\sigma \delta(E - E(\sigma))$, as

$$S(E) = \log \rho(E). \quad (3)$$

Both the energy $E$ and the entropy $S(E)$ contain extensive terms that scale with the system size, $N$. An elegant argument [10] converts Eq. (1) with $\alpha = 1$ into the statement that, for a large system, $N \to \infty$, the energy and entropy are exactly equal (up to a constant) to leading order in $N$. Thus in the thermodynamic limit, the probability distribution is indeed poised near a critical point where all derivatives beyond the first of the entropy with respect to energy vanish to leading order in $N$.

The observation of Zipf’s law in myriad distributions inferred from biological data has contributed to a revival of the idea that biological systems may be poised near a phase transition [10–15]. Yet most existing mechanisms to generate Zipf’s law can produce a variety of power-law exponents $\alpha$ (see [16,17] and reference therein), have semi-stringent conditions [18], are domain-specific, or require fine-tuning to a critical point, highlighting the crucial need to understand how Zipf’s law can arise in data-driven models.

Here we present a generic mechanism that produces Zipf’s law and does not require fine-tuning. The observation motivating this new mechanism is that the correlations measured in biological data sets have multiple origins. Some of these are intrinsic to the system, while the others reflect extrinsic, unobserved sources of variation [19,20]. For example, the distributions of activities recorded from networks of neurons in the retina reflect both the intrinsic structure of the network as well as the stimuli the neurons receive [21], such as a movie of natural scenes. Likewise, in the immune system, the pathogen environment is an external source of variation that influences the observed antibody combinations. We will show that the presence of such unobserved, hidden random variables naturally leads to Zipf’s law. Unlike other mechanisms [16,18], our approach requires a large parameter (i. e., the system size, or the number of obser-
vations), with power-law behavior emerging only in the thermodynamic limit. On the other hand, our mechanism does not require fine-tuning of parameters to a point or any special statistics of the hidden variables [22]. In other words, Zipf’s law is a universal feature that emerges when marginalizing over relevant hidden variables.

A simple model — In order to understand how a hidden variable can give rise to Zipf’s law and concomitant criticality, we start by examining a simple case of conditionally independent binary spins \( \sigma_i = \pm 1 \). The spins are influenced by a hidden variable \( h \) drawn from a probability distribution \( q(h) \), which is smooth and independent of \( N \). In particular, we consider the case

\[
P(\sigma|h) = \prod_{i=1}^{N} P(\sigma_i|h) = \prod_{i=1}^{N} \frac{e^{h\sigma_i}}{2 \cosh h}.
\]

(4)

Note that our chosen form of \( P(\sigma_i|h) \) imposes no loss of generality for non-interacting binary variables. We consider a scenario where the parameter \( h \) changes rapidly compared to the duration of the experiment, so that the probability distribution of the measured data, \( \sigma \), is averaged over \( h \):

\[
P(\sigma) = \frac{1}{2^N} \int dh q(h) e^{N(hm(h) - \log \cosh h)}
\]

\[
= \frac{1}{2^N} \int dh q(h) e^{-N\mathcal{H}(m,h)},
\]

(5)

(6)

where we have defined the average magnetization \( m = \sum_i \sigma_i/N \), and the last equation defines \( \mathcal{H}(m,h) \). Note that the distribution \( P(\sigma) \) does not factorize unlike \( P(\sigma|h) \). That is, the conditionally independent spins are not marginally independent. Indeed, as in [23], a sequence of spins carries information about the underlying \( h \) and hence about other spins (e.g., a prevalence of positive spins suggests \( h > 0 \), and thus subsequent spins will also likely be positive). We note that the simple model in Eq. (6) is intimately related to the MaxEnt model constructed in [4] to match the distribution of the number of simultaneously firing retinal ganglion cells.

In the limit \( N \gg 1 \), we can approximate the integral in Eq. (6) by Laplace’s method (saddle-point approximation) to get

\[
P(\sigma) \approx 2^{-N}(q(h^*)e^{N(h^*m - \log \cosh h^*)}), \quad \tanh h^* = m.
\]

(7)

Here \( h^* \) is the maximum-likelihood estimate of \( h \) given the data, \( \sigma \). In deriving Eq. (7) we assumed that the distribution \( q(h) \) has support at \( h^* \) and is sufficiently smooth, e.g., does not depend on \( N \), so that the saddle-point over \( h \) is determined by \( \mathcal{H} \), and not by the prior. In other words, we require that the Fisher information \( \mathcal{F}(h^*) \equiv -N \frac{\partial^2 \mathcal{H}}{\partial h^2} \bigg|_{h^*} = N(1-m^2) \gg 1 \), and for the location and curvature of the saddle point to not be significantly modulated by \( q(h) \). These conditions are violated at \( m = \pm 1 \), and there is a semi-infinite range of \( h \) that could have contributed to such states. For all nonzero values of \( \mathcal{F} \), the saddle-point will eventually dominate over \( q(h) \) as \( N \to \infty \). However, the convergence is not uniform.

Substituting Eq. (6) into Eq. (7) and using the identities

\[
\tanh^{-1} m = \frac{1}{2} \log \left( \frac{1+m}{1-m} \right) \quad \text{and} \quad \cosh \left[ \tanh^{-1} m \right] = (1 - m^2)^{-1/2},
\]

we obtain the energy to leading order in \( N \):

\[
E(m) \approx -N \left[ \left( \frac{1+m}{2} \right) \log \left( \frac{1+m}{2} \right) + \left( \frac{1-m}{2} \right) \log \left( \frac{1-m}{2} \right) \right] \equiv NH(m).
\]

(8)

Here we neglected subdominant terms that come from both the prior \( q(h^*) \) and the fluctuations about the saddle point. It is worth noting that this energy considered as a function of the \( \sigma \), rather than \( m \), includes interactions of all orders, not just pairwise spin couplings.

We can also calculate the entropy \( S(m) \) associated with the magnetization \( m \). For a system of \( N \) binary spins, each state with magnetization \( m \) has \( K = N \left( \frac{1+m}{2} \right) \) up spins, and there are \( \binom{N}{K} \) such states. Using Stirling’s approximation, one finds that the entropy takes the familiar form \( S(m) = \log \binom{N}{K} \approx NH(m) \). Of course, this is the same as the energy, Eq. (8), for the system with a hidden variable \( \beta \), to leading order in \( N \).

The analytic equivalence between energy and entropy only applies when \( N \to \infty \). To verify our result for a finite \( N \), we numerically calculate \( E(m) \) from Eq. (7) with \( q(\beta) \) chosen from a variety of distribution families (e.g., Gaussian, exponential, uniform). For brevity, we only show plots for Gaussian distributions, but the others gave similar results. Figure 1 plots the entropy, \( S(m) = \log \binom{N}{K} \), vs the energy, \( E(m) \), for \( N = 100 \) conditionally independent spins, where \( q(h) \) has mean 0 and

![Figure 1: Entropy, S(m), vs energy, E(m), for N = 100 identical and conditionally independent spins. Zipf’s law (E = S) emerges as the standard deviation, s \in \{0.1, 1, 100\}, of the Gaussian distribution characterizing the hidden variable h is increased. Notice that there is a nearly perfect Zipf’s law for 2 orders of magnitude in h. The mean of q(h) is set to zero, and thus there is a two-fold degeneracy between states with magnetization m and −m.](image-url)
varying standard deviation $s \in \{0.1, 1, 100\}$. For small $s$, the hidden variable $h$ is always close to zero, there is no averaging, and all states are nearly equally (im)-probable. As $s$ increases, entropy becomes equal to energy over many decades of energies modulo an arbitrary additive constant. This holds true for two orders of magnitude of the standard deviation $s$, confirming that our mechanism does not require fine tuning.

The stable emergence in the thermodynamic limit, $N \to \infty$, with no fine-tuning, distinguishes our setup from a classic mechanism explaining $1/f$ noise in solids [18] and certain other biological systems [24]. We could have anticipated this result: if the extensive parts of the energy and entropy do not cancel, in thermodynamic limit, the magnetization will be sharply peaked around the $m$ that minimizes the free-energy, $Nf(m) = E(m) - S(m)$. Thus in order for there to be a broad distribution of magnetizations within $\{O_\nu(x)\}$ must be a constant. In other words, the observation of a broad distribution of an order parameter-like quantity in data is indicative of a Zipfian distribution.

One straightforward mechanism to produce a broad order parameter distribution for large $N$ is to couple it to a hidden fluctuating variable.

A generic model — We now show that Zipf-like criticality is a generic property of distributions with hidden variables, and is not a consequence of the specific model in Eq. [1]: In particular, it does not require the observed variables to be identical or conditionally independent, nor the fluctuating parameter(s) to be temperature-like.

Consider a probabilistic model of data, $x = (x_1, x_2, ..., x_N)$, with $M$ parameters, $g = (g_1, ..., g_M)$. Without loss of generality, [33] we can write the probability distribution in the log-linear form

$$P(x_1, x_2, ..., x_N | g) = \frac{1}{Z(g)} \exp\left[-N \sum_{\mu=1}^{M} g_\mu O_\mu(x)\right],$$

where we have defined the partition function

$$Z(g) = \int d^n x' \exp\left[-N \sum_{\mu=1}^{M} g_\mu O_\mu(x')\right].$$

If the $x_i$ are discrete, the integral is instead a summation. As an example, the fully-connected Ising model would have $g = (h, J)$, with $O_1 = -1 \sum_i x_i$ and $O_2 = -\frac{1}{2} \sum_{i<j} x_i x_j$, with each $x_i \in \{-1, 1\}$.

If the first $K$ out of the $M$ parameters are chosen to fluctuate, according to a distribution $Q(g)$, then the marginal distribution of the data, $x$, is given by

$$P(x) = \int d^K g Q(g_1, g_2, ..., g_K) e^{-NF(g,x)},$$

with $F(g;x) = \sum_{\mu=1}^{M} g_\mu O_\mu(x) + \frac{1}{2} \ln Z(g)$. If the distribution of the $K$ fluctuating variables, $Q(g)$, is sufficiently broad, as discussed after Eq. [7], we can perform a saddle-point approximation to this integral. Denote the solution to the saddle-point equations by $g^* = (g^*_1, ..., g^*_K, g_{K+1}, ..., g_M)$ [33]. Neglecting subleading terms, the saddle-point approximation to the integral yields

$$E(x) := -\frac{1}{N} \ln P(x) = \sum_{\mu} g^*_\mu O_\mu(x) + \frac{1}{N} \ln Z(g^*),$$

where $g^*$ is the solution to

$$\frac{1}{N} \frac{\partial \ln Z(g)}{\partial g_\nu} |_{g^*} = -O_\nu(x)$$

for $\nu = 1...K$. Notice that the $g^*_\mu$ are functions of the data through the $O_\mu(x)$.

We can compare the energy in Eq. [12] to the microcanonical entropy, $S(\{O_\mu(x)\})$, calculated empirically from the data. For our problem, the multi-dimensional form of the G"artner-Ellis theorem [25] states that the entropy

$$S(\{O_\mu(x)\}) = \inf_{g} \left[ \sum_{\mu} g_\mu O_\mu(x) + c(g) \right]$$

is the Legendre-Fenchel transform of the cumulant generating function, which is, aside from an unimportant constant, just minus the free-energy,

$$c(g) = \lim_{N \to \infty} N^{-1} \ln Z(g) - C,$$

where $C = \frac{1}{N} \ln \int d^n x'$. If $K = M$, Eq. [14] is identical to Eq. [12], and we have proven Zipf’s law, i.e. $S(\{O_\mu(x)\}) = E(x)$.

Even if $K < M$, if satisfying Eq. (13) for $\nu = 1...K$ automatically satisfies Eq. (13) for $\nu = K + 1...M$, then Zipf’s law will hold. For example, in the fully-connected Ising model, matching the average magnetization, $m$, automatically provides matching of the pairwise interaction term, since it’s simply $m^2/2$. In other words, Zipf’s law will hold for any form of static interactions if the expectation values of operators conjugate to the static parameters are functions of the expectation values of operators conjugate to the fluctuating parameters.

We numerically test the validity of our analytic result for finite $N$ in two systems more complex than Eq. [4]: (a) a collection of non-identical but conditionally independent spins, and (b) an Ising model with random interactions and fields. The main graph of Fig. 2 shows a Zipf plot for system (a), so that

$$P(\sigma | \beta) = \prod_{i=1}^{N} P(\sigma_i | \beta) = \prod_{i=1}^{N} e^{-\beta h_i \sigma_i} \cosh \beta \sigma_i$$

where $h_i$ are quenched, Gaussian random variables unique for each spin. In the simulations, the hidden
variable $\beta$ was drawn from a Gaussian distribution, but similar results were found for other distributions. The quenched fields $h_i$ break the symmetry between spins. In agreement with our derivation, on a log-log plot, the states generated from simulations fall on a line with slope very close to $-1$ (Fig. 2), the signature of Zipf’s law.

To verify that conditional independence is not required for this mechanism, we studied system (b) that generalizes the model in Eq. (16) to include random exchange interactions between spins:

$$P(\sigma|\beta) \propto e^{-\beta(\sum_{i}J_{ij}\sigma_{i}\sigma_{j} + \sum_{i}h_{i}\sigma_{i})},$$

(17)

where the $J_{ij}$ and $h_i$ are quenched Gaussian distributed interactions and fields, and $\beta$ is as above. As shown in Fig. 2 (inset), the data again fall on a line with slope nearly equal to $-1$.

To see our mechanism at work in data, consider a neural spike train from a single blowfly motion-sensitive neuron H1 stimulated by a time-varying motion stimulus, $v(t)$ (see [26, 27] for experimental details). We can discretize time with a resolution of $\tau$ and interpret the spike train as an ordered sequence of $N$ spins, such that $\sigma_i = \pm 1$ corresponds to the absence/presence of a spike in a time window $t \in \tau(i - 1), \tau i)$. The probability of a spike in a time window depends on $v$. However, neural refractoriness prevents two spikes from being close to each other, irrespective of the stimulus, resulting in a repulsion that does not couple to $v$. The rank-ordered plot of spike patterns produced by the neuron is remarkably close to the Zipf behavior (Fig. 3). We also simulated a refractory Poisson spike train using the same values of $v(t)$. We chose the probability of spiking (spin up) as in Eq. (4) with $h(t) = av(t)$, $a = \text{const}$, and with a hard repulsive constraint between positive spins extending over a refractory period of duration $\tau_r$. We then choose $\tau_r$ as the shortest empirical interspike interval ($\approx 2 \text{ ms}$), and set $a$ such that the magnetization (the mean firing rate) matches the data. The rank-ordered plot for this model that manifestly includes interactions uncoupled from the hidden stimulus $v(t)$ still exhibits Zipf’s law (Fig. 3).

**Discussion** — It is possible that evolution has tuned biological systems or exploited natural mechanisms of self-organization [11] to arrive at Zipf’s law. Alternatively, informative data-driven models may lie close to a critical point due to the high density of distinguishable models there [13, 28]. Our work suggests another possibility: Zipf’s law can robustly emerge due to the effects of unobserved hidden variables. While our approach is biologically motivated, it is likely to be relevant to other systems where Zipf’s law has been observed, and it will be interesting to unearth the dominant mechanisms in particular systems. For this, if a candidate extrinsic variable can be identified, such as the input stimulus to a network of neurons, its variance could be modulated experimentally as in Fig. 1. Our mechanism would expect Zipf’s law to appear only for a broad distribution of the extrinsic variable, and for $N \gg 1$ observed variables.

While our mechanism does not require fine-tuning, it
nonetheless suggests that biological systems operate in a special regime. Indeed, the system size $N$ required to exhibit Zipf’s law depends on the sensitivity of the observed $\sigma$ to the variations of the hidden variable. If the system is poorly adapted to the distribution of $h$, e.g., the mean of $q(h)$ is very large or its width is too small to cause substantial variability in $\sigma$ (as in Fig. 1, $s = 0.1$), a very large $N$ will be required. In other words, a biological system must be sufficiently adapted to the statistics of $h$ for Zipf’s law to be observed at modest system sizes. Indeed, this type of adaptation is well established in both neural and molecular systems [29–32].

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