Guesswork, large deviations and Shannon entropy

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Abstract—How hard is it guess a password? Massey showed that the Shannon entropy of the distribution from which the password is selected is a lower bound on the expected number of guesses, but one which is not tight in general. In a series of subsequent papers under ever less restrictive stochastic assumptions, an asymptotic relationship as password length grows between scaled moments of the guesswork and specific Rényi entropy was identified.

Here we show that, when appropriately scaled, as the password length grows the logarithm of the guesswork satisfies a Large Deviation Principle (LDP), providing direct estimates of the guesswork distribution when passwords are long. The rate function governing the LDP possess a specific, restrictive form that encapsulates underlying structure in the nature of guesswork. Returning to Massey’s original observation, a corollary to the Deviation Principle (LDP), providing direct estimates of the logarithm of the guesswork.

II. A LARGE DEVIATION PRINCIPLE

Consider the sequence of random variables \(\{k^{-1} \log G(W_k)\}\). Our starting point is the observation that the Shannon entropy of the most-likely word, that

\[
\lim_{k \to \infty} \frac{1}{k} \log(\log G(W_k)) = \lim_{k \to \infty} \frac{1}{k} \log P(W_k = w) = \alpha
\]

for all \(\alpha > -1\). From this, Theorem 3 deduces that the sequence \(\{k^{-1} \log G(W_k)\}\) satisfies a Large Deviation Principle (LDP) (e.g. [6]) with a rate function \(\Lambda^*\) that must possess a specific form that will have a physical interpretation: \(\Lambda^*\) is continuous where finite, can be linear on an interval \([a, b]\), for some \(a \in [0, \log(m)]\), and then must be strictly convex while finite on \([a, \log(m)]\).

In contrast to earlier results, Corollary 4 to the LDP gives direct estimates on the guesswork distribution \(P(G(W_k) = n)\) for large \(k\), suggesting the approximation

\[
P(G(W_k) = n) \approx \frac{1}{n} \exp(-k\Lambda^*(k^{-1} \log n)).
\]

As this calculation only involves the determination of \(\Lambda^*\), to approximately calculate the probability of the \(n^{th}\) most likely word in words of length \(k\) one does not have to identify the word itself, which would be computationally cumbersome, particularly for non-i.i.d. word sources.

Corollary to the LDP recovers a rôle for Shannon entropy in the asymptotic analysis of guesswork. It shows that the scaled expectation of the logarithm of the guesswork converges to specific Shannon entropy

\[
\lim_{k \to \infty} \frac{1}{k} E(\log G(W_k)) = \lim_{k \to \infty} \frac{1}{k} H(W_k),
\]

where

\[
H(W_k) := \sum_{w \in A^k} P(W_k = w) \log P(W_k = w).
\]
that the left hand side of (1) is the scaled Cumulant Generating Function (sCGF) of this sequence:

\[ \Lambda(\alpha) := \lim_{k \to \infty} \frac{1}{k} \log E \left( e^{\alpha \log G(W_k)} \right) , \]

which is shown to exist for \( \alpha > 0 \) in [2] and for \( \alpha > -1 \) in [4].

**Assumption 1:** For \( \alpha > -1 \), the sCGF \( \Lambda(\alpha) \) exists, is equal to \( \alpha \) times the specific Rényi entropy, and has a continuous derivative in that range.

We also assume the following regularity condition on the probability of the most likely word.

**Assumption 2:** The limit

\[ g_1 = \lim_{k \to \infty} \frac{1}{k} \log P(G(W_k) = 1) \]

exists in \((-\infty, 0]\). This assumption is transparently true for words constructed of i.i.d. or Markovian letters.

We first show that the sCGF exists everywhere.

**Lemma 1 (Existence of the sCGF):** Under assumptions 1 and 2 for all \( \alpha \leq -1 \)

\[ \Lambda(\alpha) = \lim_{k \to \infty} \frac{1}{k} \log P(G(W_k) = 1) = g_1 = \lim_{\beta \downarrow -1} \Lambda(\beta). \]

**Proof:** Let \( \alpha \leq -1 \) and note that

\[ \log P(G(W_k) = 1) \leq \log \sum_{i=1}^{m^k} P(G(W_k) = i)e^{\alpha}. \]

Taking \( \lim \inf_{k \to \infty} k \) with the first inequality and \( \lim \sup_{k \to \infty} k \) with the second while using the Principle of the Largest Term, [6] Lemma 1.2.15] and usual estimates on the harmonic series, we have that

\[ \lim_{k \to \infty} \frac{1}{k} \log E(e^{\alpha \log G(W_k)}) = \lim_{k \to \infty} \frac{1}{k} \log P(G(W_k) = 1) \]

for all \( \alpha \leq -1 \).

As \( \Lambda \) is the limit of a sequence of convex functions and is finite everywhere, it is continuous and therefore \( \lim_{\beta \downarrow -1} \Lambda(\beta) = \Lambda(-1). \)

Thus the sCGF \( \Lambda \) exists and is finite for all \( \alpha \), with a potential discontinuity in its derivative at \( \alpha = -1 \). This discontinuity, when it exists, will have a bearing on the nature of the rate function governing the LDP for \( \{k^{-1} \log G(W_k)\} \). Indeed, the following quantity will play a significant rôle in our results:

\[ \gamma := \lim_{\alpha \downarrow -1} \frac{d}{d\alpha} \Lambda(\alpha). \]

We will prove that the number of words with approximately equal highest probability is close to \( \exp(k\gamma) \). In the special case where the \( \{W_k\} \) are constructed of i.i.d. letters, this is exactly true and the veracity of the following Lemma can be verified directly.

**Lemma 2 (The number of most likely words):** If \( \{W_k\} \) are constructed of i.i.d. letters, then

\[ \gamma = \lim_{\alpha \downarrow -1} \frac{d}{d\alpha} \alpha R_1((1 + \alpha)^{-1}) \]

\[ = \log \{|w : P(W_1 = w) = P(G(W_1) = 1)|\}, \]

where \(|\cdot|\) indicates the number of elements in the set.

This i.i.d. result doesn’t extend directly to the non-i.i.d. case and in general Lemma 2 can only be used to establish a lower bound on \( \gamma \):

\[ \gamma = \lim_{\alpha \downarrow -1} \frac{d}{d\alpha} \Lambda(\alpha) \geq \lim_{k \to \infty} \alpha \log \lambda(\alpha)^{-1}, \]

where \( \lambda(\alpha) \) is the probability of the most likely word.

For each fixed \( k \) there is one most likely word and we have \( \log(1) = 0 \) on the right hand side of equation 4 by Lemma 2. The left hand side, however, gives \( \log(m) \). Regardless, this intuition guides our understanding of \( \gamma \), but the formal statement of it approximately capturing the number of most likely words will transpire to be

\[ g_1 = \lim_{k \to \infty} \frac{1}{k} \log \inf_{w : G(w) < \exp(k\gamma)} P(W_k = w), \]

where \( g_1 \) is defined in equation 3.

We define the candidate rate function as the Legendre-Fenchel transform of the sCGF

\[ \Lambda^*(x) := \sup_{\alpha \in \mathbb{R}} \{x \alpha - \Lambda(\alpha)\} \]

\[ = \begin{cases} 
- x - g_1 & \text{if } x \in [0, \gamma] \\
\sup_{\alpha \in \mathbb{R}} \{x \alpha - \Lambda(\alpha)\} & \text{if } x \in (\gamma, \log(m)]. 
\end{cases} \]

The LDP cannot be proved directly by Baldi’s version of the Gärtner-Ellis theorem [3][6] Theorem 4.5.20] as \( \Lambda^* \) does not have exposing hyper-planes for \( x \in [0, \gamma] \). Instead we use a combination of that theorem with the methodology described in detail in [9] where, as our random variables are bounded \( 0 \leq \log G(W_k) \leq \log(m) \), in order to prove the LDP it suffices to show that the following exist in \([0, \infty)\) for all \( x \in [0, \log m] \) and equals \( -\Lambda^*(x) \):

\[ \lim \inf_{k \to \infty} \frac{1}{k} \log P \left( \frac{1}{k} \log(G(W_k)) \in B_x(x) \right) \]

\[ = \lim \sup_{k \to \infty} \frac{1}{k} \log P \left( \frac{1}{k} \log(G(W_k)) \in B_x(x) \right), \]

where \( B_x(x) = (x - \epsilon, x + \epsilon) \).

**Theorem 3 (The large deviations of guesswork):** Under assumptions 1 and 2, the sequence \( \{k^{-1} \log G(W_k)\} \) satisfies a LDP with rate function \( \Lambda^* \).

**Proof:** To establish 4 we have separate arguments depending on \( x \). We divide \([0, \log(m)]\) into two parts: \([0, \gamma]\) and \((\gamma, \log(m)]\). Baldi’s upper bound holds for any \( x \in [0, \log(m)] \). Baldi’s lower bound applies for any \( x \in (\gamma, \log(m)] \) as \( \Lambda^* \) is continuous and, as \( \Lambda(\alpha) \) has a continuous
derivative for $\alpha > -1$, it only has a finite number of points without exposing hyper-planes in that region. For $x \in [0, \gamma]$, however, we need an alternate lower bound.

Consider $x \in [0, \gamma]$ and define the sets

$$K_k(x, \epsilon) := \{ w \in k^k : k^{-1} \log G(w) \in B_\epsilon(x) \},$$

letting $|K_k(x, \epsilon)|$ denote the number of elements in each set. We have the bound

$$|K_k(x, \epsilon)| \inf_{w \in K_k(x, \epsilon)} P(W_k = w) \leq P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x)\right).$$

As $|e^{k(x-\epsilon)}| \leq |K_k(x, \epsilon)| \leq \lceil e^{k(x+\epsilon)} \rceil$, we have that

$$x = \lim_{\epsilon \to 0} \lim_{k \to \infty} \frac{1}{k} \log |K_k(x, \epsilon)|. \tag{7}$$

By Baldi’s upper bound, we have that

$$\lim_{\epsilon \to 0} \lim_{k \to \infty} \frac{1}{k} \log P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x)\right) \leq x + g_1.$$ 

Thus to complete the argument, for the complementary lower bound we need to show that for any $x \in [0, \gamma]$

$$\lim_{\epsilon \to 0} \lim_{k \to \infty} \inf_{w \in K_k(x, \epsilon)} \frac{1}{k} \log P(W_k = w) = g_1.$$ 

If $\Lambda^*(x) < \infty$ for some $x > \gamma$, then for $\epsilon > 0$ sufficiently small let $x^\ast$ be such that $\Lambda^*(x^\ast) < \infty$ and $x^\ast - \epsilon > \max(\gamma, x + \epsilon)$. Then by Baldi’s lower bound, which applies as $x^\ast \in (\gamma, \log(m))$, we have

$$-\inf_{y \in B_\epsilon(x^\ast)} \Lambda^*(y) \leq \liminf_{k \to \infty} \frac{1}{k} \log P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x^\ast)\right).$$

Now

$$P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x^\ast)\right) \leq \inf_{y \in B_\epsilon(x^\ast)} \Lambda^*(y) \leq \liminf_{k \to \infty} \frac{1}{k} \log P(W_k = w)$$

for all such $x^\ast$, $x$. Taking limits as $\epsilon \downarrow 0$ and then limits as $x^\ast \downarrow \gamma$ we have

$$-\lim_{x^\ast \downarrow \gamma} \Lambda^*(x^\ast) \leq \gamma + \liminf_{k \to \infty} \frac{1}{k} \log P(W_k = w),$$

but $\lim_{x^\ast \downarrow \gamma} \Lambda^*(x^\ast) = -\gamma - g_1$ so that

$$\lim_{\epsilon \to 0} \liminf_{k \to \infty} \frac{1}{k} \log P(W_k = w) = g_1,$$

as required.

Only one case remains: if $\Lambda^*(x) = \infty$ for all $x > \gamma$, then we require an alternative argument to ensure that

$$\liminf_{k \to \infty} \inf_{w \in K_k(x, \epsilon)} \frac{1}{k} \log P(W_k = w) = g_1.$$ 

This situation happens if, in the limit, the distribution of words is near uniform on the set of all words with positive probability. Thus define

$$\mu := \limsup_{k \to \infty} \frac{1}{k} \log |\{ w : P(W_k = w) > 0 \}|.$$ 

As $\Lambda^*(x) = \infty$ for all $x > \gamma$, $\mu \leq \gamma$. To see $\gamma = \mu$, note that $\gamma = \lim_{\alpha \downarrow 1} \Lambda^*(\alpha) \leq \Lambda^*(0)$. As both $\Lambda(\alpha)$ and $\alpha R_k((1 + \alpha)^{-1})$ are finite and differentiable in a neighborhood of $0$, by [7, Theorem 25.7]

$$\Lambda^*(0) = \lim_{k \to \infty} \frac{1}{k} \frac{d}{d\alpha}\alpha R_k((1 + \alpha)^{-1})|_{\alpha=0} = \lim_{k \to \infty} \frac{1}{k} \log(H(W_k)).$$

and $\log_{k \to \infty} k^{-1} H(W_k) \leq \mu$. Thus $\gamma = \mu$ and, due to convexity, $\Lambda$ is linear with slope $\mu$ on $\alpha \in (-1, 0]$. As $\Lambda(0) = 0$, using Lemma[1] we have that $g_1 = -\mu$. Let $x < \mu$ and consider

$$l = \limsup_{k \to \infty} \sup_{w \in K_k(x, \epsilon, \mu)} \frac{1}{k} \log P(W_k = w) \leq \liminf_{k \to \infty} \inf_{w \in K_k(x, \epsilon, \mu)} \frac{1}{k} \log P(W_k = w).$$

We shall assume that $l < g_1$ and show this results in a contradiction. Let $\epsilon < \min(g_1 - l, \mu - x)/2$, then there exists $N_\epsilon$ such that

$$\sum_{w \in k^k} P(W_k = w) \leq e^{k(x+\epsilon)} e^{k(g_1+\epsilon)} e^{k(\mu+\epsilon)} = e^{k(-\mu+x+2\epsilon)} + e^{k(g_1+l+2\epsilon)},$$

for all $k > N_\epsilon$, but this is strictly less than 1 for $k$ sufficiently large and thus $l = g_1$. Finally, for $x = \mu$, and $\epsilon > 0$, note that we can decompose $[0, \log(m)]$ into three parts, $[0, \mu - \epsilon] \cup (\mu - \epsilon, \mu + \epsilon) \cup [\mu + \epsilon, \log(m)]$, where the scaled probability of the guesswork being in either the first or last set is decaying, but

$$0 = \lim_{k \to \infty} \frac{1}{k} \log(P\left(\frac{1}{k} \log G(W_k) \in [0, \log(m)]\right))$$

and so the result follows from an application of the principle of the largest term.

Thus for any $x \in [0, \log(m)]$,

$$\lim_{\epsilon \to 0} \liminf_{k \to \infty} \frac{1}{k} \log P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x)\right) = \lim_{\epsilon \to 0} \limsup_{k \to \infty} \frac{1}{k} \log P\left(\frac{1}{k} \log G(W_k) \in B_\epsilon(x)\right) = -\Lambda^*(x)$$

and the LDP is proved. 

In establishing the LDP, we have shown that any rate function that governs such an LDP must have the form of a straight line in $[0, \gamma]$ followed by a strictly convex function. The initial straight line comes from all words that are, in an asymptotic sense, of greatest likelihood.
While the LDP is for the sequence \( \{k^{-1} \log G(W_k)\} \), it can be used to develop the more valuable direct estimate of the distribution of each \( G(W_k) \) found in equation 2. The next corollary provides a rigorous statement, but an intuitive, non-rigorous argument for understanding the result therein is that from the LDP we have the approximation that for large \( k \)

\[
dP\left( \frac{1}{k} \log G(W_k) = x \right) \approx \exp(-k \Lambda^*(x)).
\]

As for large \( k \) the distribution of \( k^{-1} \log G(W_k) \) and \( G(W_k)/k \) are ever closer to having densities, using the change of variables formula gives

\[
dP\left( \frac{1}{k} G(W_k) = x \right) = \frac{1}{k x} dP\left( \frac{1}{k} \log G(W_k) = x \right) \approx \frac{1}{k x} \exp\left(-k \Lambda^*\left(\frac{1}{k} \log(kx)\right)\right).
\]

Finally, the substitution \( kx = n \) gives the approximation in equation 2. To make this heuristic precise requires distinct means, explained in the following corollary.

**Corollary 4 (Direct estimates on guesswork):** Recall the definition

\[
K_k(x, \epsilon) := \{w \in \mathbb{A}^k : k^{-1} \log G(w) \in B_\epsilon(x)\}.
\]

For any \( x \in [0, \log(m)] \) we have

\[
\lim \inf_{x \to 0} \lambda \inf_{k \to \infty} \frac{1}{k} \log \inf_{w \in K_k(x, \epsilon)} P(W_k = w)
\]

\[
= \lim \sup_{x \to 0} \lambda \sup_{k \to \infty} \frac{1}{k} \log \sup_{w \in K_k(x, \epsilon)} P(W_k = w)
\]

\[
= -(x + \Lambda^*(x)).
\]

**Proof:** We show how to prove the upper bound as the lower bound follows using analogous arguments, as do the edge cases. Let \( x \in (0, \log(m)) \) and \( \epsilon > 0 \) be given. Using the monotonicity of guesswork

\[
\lim \sup_{k \to \infty} \frac{1}{k} \log \sup_{w \in K_k(x, \epsilon)} P(W_k = w)
\]

\[
\leq \lim \inf_{k \to \infty} \frac{1}{k} \log \inf_{w \in K_k(x-2\epsilon, \epsilon)} P(W_k = w).
\]

Using the estimate found in Theorem 3 and the LDP provides an upper bound on the latter:

\[
(x - 3\epsilon) + \lim \inf_{k \to \infty} \frac{1}{k} \log \inf_{w \in K_k(x-2\epsilon, \epsilon)} P(W_k = w)
\]

\[
\leq \lim \inf_{k \to \infty} \frac{1}{k} \log \left( \frac{1}{k} \log(G(W_k)) \right) \in B_\epsilon(x - 2\epsilon)
\]

\[
\leq \lim \sup_{k \to \infty} \frac{1}{k} \log \left( \frac{1}{k} \log(G(W_k)) \right) \in [x - 3\epsilon, x - \epsilon]
\]

\[
\leq - \inf_{x \in [x - 3\epsilon, x - \epsilon]} \Lambda^*(x).
\]

Thus

\[
\lim \sup_{k \to \infty} \frac{1}{k} \log \sup_{w \in K_k(x, \epsilon)} P(W_k = w)
\]

\[
\leq -x + 3\epsilon - \inf_{x \in [x - 3\epsilon, x - \epsilon]} \Lambda^*(x).
\]

Thus the upper-bound follows taking \( \epsilon \downarrow 0 \) and using the continuity when finite of \( \Lambda^* \).

Unpeeling limits, this corollary shows that when \( k \) is large the probability of the \( n^{th} \) most likely word is approximately \( 1/n \exp(-k \Lambda^*(k^{-1} \log n)) \), without the need to identify the word itself. This justifies the approximation in equation 2, whose complexity of evaluation does not depend on \( k \). We demonstrate its merit by example in Section III.

Before that, as a corollary to the LDP we find the following rôle for the specific Shannon entropy. Thus, although Massey established that for a given word length the Shannon entropy is only a lower bound on the guesswork, for growing password length the specific Shannon entropy determines the linear growth rate of the expectation of the logarithm of guesswork.

**Corollary 5 (Shannon entropy and guesswork):** Under assumptions [1] and [2]

\[
\lim_{k \to \infty} \frac{1}{k} E(\log(G(W_k))) = \lim_{k \to \infty} \frac{1}{k} H(W_k),
\]

the specific Shannon entropy.

**Proof:** Note that \( \Lambda^*(x) = 0 \) if and only if \( x = \Lambda'(0) = \lim k^{-1} H(W_k) \), by arguments found in the proof of Theorem 3. The weak law then follows by concentration of measure, e.g. [10].

### III. Examples

**I.i.d. letters.**

Assume words are constructed from i.i.d. letters. Let \( W_k \) take values in \( \mathbb{A} = \{1, \ldots, m\} \) and assume \( P(W_1 = i) \geq P(W_1 = j) \) if \( i \leq j \). Then from [2] and Lemma 1 we have that

\[
\Lambda(\alpha) = \begin{cases} (1 + \alpha) \log \sum_{w \in \mathbb{A}} P(W_1 = w)^{1/(1+\alpha)} & \text{if } \alpha > -1 \\ \log P(W_1 = 1) & \text{if } \alpha \leq -1. \end{cases}
\]

From Lemma 2 we have that

\[
\gamma = \lim_{\alpha \to -1} \Lambda'(\alpha) \in [0, \log(2), \ldots, \log(m)]
\]

and no other values are possible. Unless the distribution of \( W_1 \) is uniform, \( \Lambda' \) does not have a closed form for all
distribution on a Markov chain with transition matrix $P$ has not increased.

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to make them comparable for distinct

can clearly be seen. Rescaling the guesswork and probabilities

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1

words of equal highest

definitely only describes the number of words of equal highest
likelihood when $k$ is large as the initial distribution of the
Markov chain plays no rôle in $\gamma$’s evaluation.

The case where $\gamma = \log(2)$ occurs when $p_{1,1} = p_{2,2} = 1/2$. The most interesting case is when there are approximately $\phi^k$ approximately equally most likely words. This occurs if $p_{1,1} = \sqrt{p_{1,2}p_{2,1}} > p_{2,2}$. For large $k$, words of near-maximal probability have the form of a sequence of 1s, where a 2 can be inserted anywhere so long as there is a 1 between it and any other 2s. A further sub-exponential number of aberrations are allowed in any given sequence. For example, with an equiprobable initial distribution and $k = 4$ there are 8 most likely words ($1111, 1112, 1121, 1211, 1212, 2111, 2121, 2112$) and $\phi^4 \approx 6.86$.

Figure 3 gives plots of $\Lambda^*(x)$ versus $x$ illustrating the full range of possible shapes that rate functions can take: linear, linear then strictly convex, or strictly convex, based on the transition matrices

\[
\begin{pmatrix}
0.5 & 0.5 \\
0.5 & 0.5
\end{pmatrix},
\begin{pmatrix}
0.6 & 0.4 \\
0.9 & 0.1
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
0.85 & 0.15 \\
0.15 & 0.85
\end{pmatrix}
\]

respectively.

REFERENCES


