## On Turing's formula and the estimation of the missing mass

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# Part I: Estimation of the Missing Mass 

Joint work with Z. Zhang

## Bird Example

Consider the bird population in a particular location ...

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- Unknown species proportions: $P=\left\{p_{1}, p_{2}, \cdots\right\}$
- A sample of $n=2000$ is taken.
- Counts: $x_{1}=300, x_{2}=200, \cdots$
- $\hat{p}_{1}=0.15, \hat{p}_{2}=0.10, \cdots$ estimating $p_{1}, p_{2}, \cdots$


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- A2: An answer is given by Turing's formula.
$T_{0, n}=\frac{\# \text { of species occurring exactly once in the sample }}{n}$.


## Intuition

Turing's formula estimation the probability of seeing a new species by

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## Notation

Let

- $\mathcal{A}=\left\{a_{1}, a_{2}, \ldots\right\}=$ an at most countable alphabet.
- $P=\left\{p_{a}: a \in \mathcal{A}\right\}$ the associated probability distribution, where $p_{a} \in[0,1]$ and $\sum_{a \in \mathcal{A}} p_{a}=1$.
- $\mathcal{S}=\left\{a \in \mathcal{A}: p_{a}>0\right\}=$ the support of $P$.


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- $\mathcal{S}=\left\{a \in \mathcal{A}: p_{a}>0\right\}=$ the support of $P$.

Let $X_{1}, \ldots, X_{n}$ be independent and identically distributed $\mathcal{A}$-valued random variables, with distribution $P$.

- $L_{n}(a)=\sum_{i=1}^{n} \mathbf{1}\left\{X_{i}=a\right\}$ - the sample counts of $a \in \mathcal{A}$;
- $\hat{p}_{a}=L_{n}(a) / n$ - the sample proportion of $a \in \mathcal{A}$.
- $K_{r, n}=\sum_{a \in \mathcal{A}} 1_{\left[L_{n}(a)=r\right]}, r=0,1, \ldots, n$.


## Missing Mass

The missing mass is the total probability associated with the letters not covered in the sample, it is given by

$$
M_{0, n}=\sum_{a \in \mathcal{A}} p_{a} \mathbf{1}\left\{L_{n}(a)=0\right\}
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$$

Note that this is not a parameter or a statistic. It depends on both unknown parameters and the sample.

## Turing's Formula

A "good" estimator of the missing mass

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M_{0, n}=\sum_{a \in \mathcal{A}} p_{a} \mathbf{1}\left\{L_{n}(a)=0\right\}
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is provided by Turing's formula
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This formula was first introduced in Good (1953), where the results were largely credited to Alan Turing.

## Bias of Turing's Formula

$$
\mathbb{E}\left[T_{0, n}-M_{0, n}\right]=\sum_{a \in \mathcal{A}} p_{a}^{2}\left(1-p_{a}\right)^{n-1}>0 .
$$

Thus, for large $n$,

$$
\mathbb{E}\left[T_{0, n}-M_{0, n}\right] \approx 0
$$

## Consistency of Turing's Formula

We always have

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T_{0, n}-M_{0, n} \xrightarrow{p} 0 .
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However,

$$
M_{0, n} \xrightarrow{p} 0, \quad T_{0, n} \xrightarrow{p} 0, \text { as } n \rightarrow \infty
$$

## Consistency in Relative Error

Ohannessian and Dahleh (2012) suggested that it is more meaningful to consider consistency in relative error:

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\frac{T_{0, n}-M_{0, n}}{M_{0, n}} \xrightarrow{p} 0 .
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This does not hold for all distributions.
Ben-Hamou et al. (2017) gave sufficient conditions when this holds.

## Asymptotic normality

We consider the related problem of asymptotic normality. This allows not just for estimation, but for statistical inference.

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Asymptotic normality for Turing's formula was considered in Esty (1983), Zhang and Huang (2008), Zhang and Zhang (2009), and Grabchak and Zhang (2017).

## Main Theorem

Let $g_{n}$ be a deterministic sequence of positive numbers with

$$
\limsup _{n \rightarrow \infty} \frac{g_{n}}{n^{1-\beta}}<\infty \text { for some } \beta \in(0,1 / 2)
$$

If there are constants $c_{1}>0$ and $c_{2} \geq 0$ with

$$
\lim _{n \rightarrow \infty} \frac{g_{n}^{2}}{n} \mathbb{E}\left[T_{0, n}\right]=c_{1} \text { and } \lim _{n \rightarrow \infty} g_{n}^{2} \sum_{a \in \mathcal{A}} p_{a}^{2} e^{-n p_{a}}=c_{2}
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$$

then

$$
h_{n}\left(\frac{T_{0, n}-M_{0, n}}{M_{0, n}}\right) \xrightarrow{d} N\left(0, c_{1}+c_{2}\right) .
$$

where $h_{n}=\mathbb{E}\left[M_{0, n}\right] g_{n}$

## Corollary

In practice, we don't know $g_{n}$, but so long as it exists, it and the other parameters can be estimated.

Corollary. If the conditions of the Theorem are satisfied, then

$$
\frac{K_{1, n}}{\sqrt{K_{1, n}+2 K_{2, n}}}\left(\frac{T_{0, n}-M_{0, n}}{M_{0, n}}\right) \xrightarrow{d} N(0,1)
$$

where

$$
K_{r, n}=\sum_{a \in \mathcal{A}} \mathbf{1}\left\{L_{n}(a)=r\right\}
$$

## Confidence Intervals

If $\frac{K_{1, n}}{2 K_{2, n}}$ is not very close to 0 , then an approximate $(1-\alpha) 100 \%$ confidence interval
$\frac{K_{1, n}^{2} / n}{K_{1, n}+z_{\alpha / 2} \sqrt{K_{1, n}+2 K_{2, n}}} \leq M_{0, n} \leq \frac{K_{1, n}^{2} / n}{K_{1, n}-z_{\alpha / 2} \sqrt{K_{1, n}+2 K_{2, n}}}$
where $z_{\alpha / 2}$ is a number with $P\left(Z>z_{\alpha / 2}\right)=\alpha / 2$.

## Consistency

Corollary. If the conditions of the Theorem are satisfied, then

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Our conditions appear to be different from the ones given in Ben-Hamou et al. (2017)

## The Counting Function

To talk about tails of distributions on an alphabet, Karlin (1967) introduced the counting function $\nu:[0,1] \rightarrow \mathbb{N}$, defined by

$$
\nu(\varepsilon)=\sum_{a \in \mathcal{A}} 1\left\{p_{a} \geq \varepsilon\right\}
$$

## Facts:

1. $\nu$ is non-increasing with $\varepsilon$
2. For all $0<\varepsilon \leq 1, \nu(\varepsilon) \leq \varepsilon^{-1}$
3. $\varepsilon \nu(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow 0$

## Regularly Varying Distributions

A discrete distribution $P$ is said to be regularly varying with index $\alpha \in[0,1]$ if

$$
\nu(\varepsilon)=\varepsilon^{-\alpha} \ell(1 / \varepsilon),
$$

where $\ell$ is a slowly varying function, i.e.

$$
\lim _{x \rightarrow \infty} \frac{\ell(x t)}{\ell(x)}=1, \text { for any } t>0
$$

In this case we write $P \in \mathcal{R} \mathcal{V}_{\alpha}(\ell)$. This definition is due to Karlin (1967), see Gnedin et al. (2007) for a recent review.

## Regularly Varying Distributions

Fact: Assume that $\mathcal{A}=\mathbb{N}$. $P \in \mathcal{R} \mathcal{V}_{\alpha}(\ell)$ with $\alpha \in(0,1)$ if and only if

$$
p_{k} \sim \ell^{*}(k) k^{-1 / \alpha} \text { as } k \rightarrow \infty,
$$

where $\ell^{*}$ is a slowly varying function, in general, different from $\ell$.

## Results for Regularly Varying Distributions

Proposition. If $P \in \mathcal{R} \mathcal{V}_{\alpha}(\ell)$ for some $\alpha \in(0,1)$ then, the assumptions of the Theorem hold and

$$
\kappa_{\alpha} n^{\alpha / 2}[\ell(n)]^{1 / 2}\left(\frac{T_{0, n}-M_{0, n}}{M_{0, n}}\right) \xrightarrow{d} N(0,1) \text { as } n \rightarrow \infty,
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where $\kappa_{\alpha}=\sqrt{\frac{\alpha \Gamma(1-\alpha)}{2-\alpha}}$.

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where $\kappa_{\alpha}=\sqrt{\frac{\alpha \Gamma(1-\alpha)}{2-\alpha}}$.
A similar result holds for $\alpha=1$, but with a somewhat different scaling.

## Case $\alpha=0$

When $\alpha=0$ the distributions may no longer be heavy tailed and the results of the Theorem need not hold.

Ohannessian and Dahleh (2012) showed that consistency in relative error cannot hold for certain $\mathcal{R} \mathcal{V}_{0}$ distributions.

## Extension: rth order Turing Formula

For any $0 \leq r \leq n-1$ we define the occupancy probabilities by

$$
M_{r, n}=\sum_{a \in \mathcal{A}} p_{a} \mathbf{1}\left\{L_{n}(a)=r\right\}
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and the occupancy counts by

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$$

We can estimate $M_{r, n}$ by the $r$ th order Turing's formula

$$
T_{r, n}=\frac{r+1}{n-r} K_{r+1, n}
$$

and our results can be extended to this case

# Part II: Expectation of the Missing Mass 

Joint work with G. Decrouez and Q. Paris

## Main Objects

For $0 \leq r \leq n$, the occupancy counts $K_{r, n}$ are defined by

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The missing mass is $M_{0, n}$.

## Statement of Problem

Our Goal: To understand the finite sample properties of $\mathbb{E} K_{r, n}$ and $\mathbb{E} M_{r, n}$.

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$$

For this reason we only focus on $\mathbb{E} M_{r, n}$
This problem was previously studied in Ohannessian and Dahleh (2010) and Berend and Kontorovich (2012) for the case $r=0$.

## Statement of Problem

In short, we study the object

$$
\mathbb{E} M_{r, n}=\binom{n}{r} \sum_{a \in \mathcal{A}} p_{a}^{r+1}\left(1-p_{a}\right)^{n-r}
$$

## Upper Bounds

Theorem
For any $n \geq 1$ and any $0 \leq r \leq n-1$, we have

$$
\mathbb{E} M_{r, n} \leq \inf _{0 \leq \varepsilon \leq 1}\left\{\varphi_{r, n}^{+}(\varepsilon)+\psi_{r, n}^{+}(\varepsilon)\right\}
$$

where

$$
\begin{aligned}
\varphi_{r, n}^{+}(\varepsilon) & =\frac{c(r) \nu(\varepsilon)}{n} \\
\psi_{r, n}^{+}(\varepsilon) & =2^{1+r}\binom{n}{r} \int_{0}^{\varepsilon} \nu\left(\frac{u}{2}\right) u^{r}\left(1-\frac{u}{2}\right)^{n-r} \mathrm{~d} u \\
c(r) & = \begin{cases}e^{-1} & \text { if } r=0 \\
\frac{(1+r)^{2+r}}{r!} e^{-\frac{1+r}{2}} & \text { if } 1 \leq r \leq n-1\end{cases}
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\end{aligned}
$$

In many situations, a relevant choice of $\varepsilon$ yields explicit and, as far as we know, new bounds.

## Finite Support

Corollary. Suppose that $\mathcal{S}$ is finite. Then, for all $n \geq 1$ and all $0 \leq r \leq n-1$,

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\mathbb{E} M_{r, n} \leq \frac{c(r)|\mathcal{S}|}{n}
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\mathbb{E} M_{r, n} \leq \frac{c(r)|\mathcal{S}|}{n}
$$

When we take $r=0$ we recover the bound for the expected missing mass

$$
\mathbb{E} M_{0, n} \leq \frac{|\mathcal{S}|}{n e}
$$

provided by Berend and Kontorovich (2012).

## Regular Variation

Fact : $\nu(\varepsilon)=\varepsilon^{-\alpha} \ell\left(\frac{1}{\varepsilon}\right) \Rightarrow \mathbb{E} M_{r, n} \underset{n \rightarrow \infty}{\sim} \frac{\alpha \Gamma(1+r-\alpha)}{r!} \frac{\ell(n)}{n^{1-\alpha}}$

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## Corollary.

$$
\nu(\varepsilon) \leq \varepsilon^{-\alpha} \ell\left(\frac{1}{\varepsilon}\right) \quad \Rightarrow \quad \mathbb{E} M_{r, n} \leq c(\alpha, r) \frac{\ell(n)}{n^{1-\alpha}},
$$

where

$$
c(\alpha, r)=c(r)+\frac{4^{1+r}}{r!}(1+r)^{1+r-\alpha} \int_{0}^{1 / 2} u^{r-\alpha} e^{-u} \mathrm{~d} u
$$

where $\ell$ is nondecreasing.

## Regular Variation: Lower Bounds

Fact : $\nu(\varepsilon)=\varepsilon^{-\alpha} \ell\left(\frac{1}{\varepsilon}\right) \Rightarrow \mathbb{E} M_{r, n} \underset{n \rightarrow \infty}{\sim} \frac{\alpha \Gamma(1+r-\alpha)}{r!} \frac{\ell(n)}{n^{1-\alpha}}$

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## Corollary.

$$
\nu(\varepsilon) \geq \varepsilon^{-\alpha} \ell\left(\frac{1}{\varepsilon}\right) \quad \Rightarrow \quad \mathbb{E} M_{r, n} \geq c_{1}(\alpha, r) \frac{\ell(n)}{n^{1-\alpha}},
$$

where $\ell$ is nondecreasing.

## Application: Bounds in Probability

Concentration inequalities for the missing mass have been studied in McAllester and Ortiz (2003), Ohannessian and Dahleh (2012), and Ben-Hamou et al. (2017).

These can combined with our bounds to get bounds in probability.

## Application: Bounds in Probability

Example: Assume that, for some $\alpha \in(0,1)$,

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For all $t>0$,

$$
\mathbb{P}\left(m_{0, n}^{-}(t, \alpha) \leq M_{0, n} \leq m_{0, n}^{+}(t, \alpha)\right) \geq 1-2 e^{-t}
$$

where

$$
\begin{aligned}
& m_{0, n}^{-}(t, \alpha)=\frac{\left(2^{\alpha}-1\right) \gamma(1-\alpha, 2)}{32} \frac{C_{\alpha}^{\alpha}}{n^{1-\alpha}}-\sqrt{\frac{2 t}{n e}} \\
& m_{0, n}^{+}(t, \alpha)=\left(\frac{1}{e}+4 \gamma\left(1-\alpha, \frac{1}{2}\right)\right) \frac{C_{\alpha}^{\alpha}}{n^{1-\alpha}}+\sqrt{\frac{t}{n}}
\end{aligned}
$$

## Part III: Simpson's Indices

Joint work with L. Cao and Z. Zhang

## Simpson's Index

Simpson (1949), introduced a bio-diversity index

$$
\zeta_{1}=\sum_{a \in \mathcal{A}} p_{a}\left(1-p_{a}\right)
$$

It is sometimes called Simpson's index or the Gini-Simpson index.

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To estimate the diversity of an eco-system, we can estimate $\zeta_{1}$.

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\sum_{a \in \mathcal{A}} \hat{p}_{a}\left(1-\hat{p}_{a}\right),
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$$

but this is a biased estimator.

## Simpson's Index

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$$
\zeta_{1}=\sum_{a \in \mathcal{A}} p_{a}\left(1-p_{a}\right)
$$

Instead Simpson (1949) suggested the unbiased estimator

$$
Z_{1}=\frac{n}{n-1} \sum_{a \in \mathcal{A}} \hat{p}_{a}\left(1-\hat{p}_{a}\right)
$$

## Generalized Simpson's Indices

We now introduce a more general class of indices due to Zhang and Zhou (2010).

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A Generalized Simpson's Index of order $v \in \mathbb{N}$ is

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A Generalized Simpson's Index of order $v \in \mathbb{N}$ is

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\zeta_{v}=\sum_{a \in \mathcal{A}} p_{a}\left(1-p_{a}\right)^{v}=\mathbb{E} M_{0, v}
$$

Fact: The collection $\left\{\zeta_{v}: n=1,2, \ldots\right\}$ determines the distributions $\left\{p_{1}, p_{2}, \ldots\right\}$ up to permutation.

## Generalized Simpson's Indices

Zhang and Zhou (2010) showed that an unbiased estimator of the Generalized Simpson's Indices of order $v=1,2, \ldots,(n-1)$

$$
\zeta_{v}=\sum_{a \in \mathcal{A}} p_{a}\left(1-p_{a}\right)^{v}
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is given by

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Z_{v}=\sum_{a \in \mathcal{A}} \hat{p}_{a} \prod_{j=1}^{v}\left(1-\frac{n \hat{p}_{a}-1}{n-j}\right) .
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Fact: When $v=n-1, Z_{n-1}=T_{0, n}$ reduces to Turing's formula.

## Generalized Simpson's Indices

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\frac{\sqrt{n}\left(Z_{v}-\zeta_{v}\right)}{\hat{\sigma}_{v}} \xrightarrow{d} N(0,1),
$$

where

$$
\begin{aligned}
\hat{\sigma}_{v}^{2}= & \sum_{a \in \mathcal{A}} \hat{p}_{a}\left(1-\hat{p}_{a}\right)^{2 v-2}\left(1-v \hat{p}_{a}-\hat{p}_{a}\right)^{2} \\
& -\left(\sum_{a \in \mathcal{A}} \hat{p}_{a}\left(1-\hat{p}_{a}\right)^{v-1}\left(1-v \hat{p}_{a}-\hat{p}_{a}\right)\right)^{2}
\end{aligned}
$$

## An Application to Linguistics

In 1985 the following poem was discovered. It begins...

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Shall I die? Shall I fly<br>Lover's baits and deceits sorrow breeding?<br>Shall I tend? Shall I send?<br>Shall I sue, and not rue my proceeding?<br>In all duty her beauty<br>Binds me her servant for ever.<br>If she scorn, I mourn,<br>I retire to despair, joining never.

## Who wrote this poem?

On it the author's name was written: William Shakespeare.
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Did Shakespeare really write the poem?
Many literary scholars have debated this question.
As have some statisticians, see e.g. Thisted and Efron (1987).

## Our Methodology

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Let $P=\left\{p_{1}, p_{2}, \ldots\right\}$ be the relative frequencies with which an author uses the words.

We can summarize the information in $P$ by using

$$
\zeta_{v}=\sum_{a \in \mathcal{A}} p_{a}\left(1-p_{a}\right)^{v}
$$

for various values of $v$.

## Our Methodology

To test the authorship of "Shall I Die?" we:

- Estimate $\zeta_{1}, \ldots, \zeta_{200}$ for the poem
- Estimate $\zeta_{1}, \ldots, \zeta_{200}$ for a corpus consisting of Shakespeare's sonnets
- Plot the difference and a confidence interval


## Comparison of Sonnets and Sonnets From Plays



95\% CI for sonnets from plays


## Comparison of Sonnets and The Raven

Profile for 'The Raven'


95\% Cl for 'The Raven'


## Comparison of Sonnets and Philip Sidney's Astrophel and Stella

Profile for 'Astrophel and Stella'


95\% CI for 'Astrophel and Stella'


## Comparison of Sonnets and Shall I Die

Profile for 'Shall I Die?'


95\% Cl for 'Shall I Die?'


## Bibliography

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M. Grabchak, L. Cao, and Z. Zhang (2017). Authorship Attribution Using Diversity Profiles. To appear in Journal of Quantitative Linguistics, DOI: 10.1080/09296174.2017. 1343268.
M. Grabchak and Z. Zhang (2017). Asymptotic Properties of Turing's Formula in Relative Error. Machine Learning, 106(11):1771-1785.

## Simulations

To better understand how Turing's formula works, we perform simulations. We measure performance by:

1. Expected absolute error:

$$
\mathbb{E}\left|T_{0, n}-M_{0, n}\right|
$$

2. Expected relative error:

$$
\mathbb{E}\left|\frac{T_{0, n}-M_{0, n}}{M_{0}}\right|
$$

## Simulations for Poisson

Estimated Absolute Relative Error For Poisson


Estimated Relative Error For Poisson

short-dashes: $\lambda=1$, long-dashes: $\lambda=5$, solid: $\lambda=10$

## Simulations for Geometric

Estimated Expected Absolute Error For Geometric


Estimated Expected Relative Error For Geometric

short-dashes: $p=.7$, long-dashes: $p=.5$, solid: $p=.1$

## Simulations for Discrete Pareto

Estimated Expected Absolute Error For Discrete Pareto


Estimated Expected Relative Error For Discrete Pareto

short-dashes: $\alpha=10$, long-dashes: $\alpha=5$, solid: $\alpha=1$

## Conclusions From Simulations

1. Absolute error decays quickly for all distributions. But, as we have seen, this may not be relevant.
2. Relative error is smaller for heavier tailed distributions. Only goes to zero for heavy tailed distributions.

## Extension: Metric Spaces

- $(E, d)$ is a metric space
- $P$ is a probability distribution on $E$
- $X_{1}, \ldots, X_{n}$ are a random sample of $E$-valued random variables with common distribution $P$


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Since $E$ may not be discrete, we need to define analogues of occupancy probabilities, $M_{r, n}$, and the counting function $\nu$.

## Extension: Metric Spaces

Occupancy Probabilities - For $\delta>0, n \geq 1$, and $x \in E$,

$$
L_{n}^{\delta}(x):=\sum_{i=1}^{n} \mathbf{1}\left\{X_{n} \in B_{x, \delta}\right\}
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Definition. For $n \geq 1$ and $0 \leq r \leq n$,

$$
M_{n, r}^{\delta}=\mathbb{P}\left(L_{n}^{\delta}\left(X_{n+1}\right)=r \mid X_{1}, \ldots, X_{n}\right)=\int_{E} 1\left\{L_{n}^{\delta}(x)=r\right\} P(\mathrm{~d} x)
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Fact: If $P$ has a discrete support with no accumulation point, then

$$
M_{n, r}^{\delta} \underset{\delta \rightarrow 0+}{\longrightarrow} M_{n, r}
$$

## Extension: Metric Spaces

$\delta$-Counting Function: For $\delta>0$ define

$$
\mathcal{L}_{\delta}(\varepsilon)=\left\{x \in E: P\left(B_{x, \delta}\right) \geq \varepsilon\right\}
$$

and

$$
\nu_{\delta}(\varepsilon)=\int_{\mathcal{L}_{\delta}(\varepsilon)} P\left(B_{x, \delta}\right)^{-1} P(\mathrm{~d} x)
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$$

Theorem. If $P$ has a discrete support with no accumulation point, then for any $\varepsilon \in(0,1]$,

$$
\nu_{\delta}(\varepsilon) \underset{\delta \rightarrow 0+}{\longrightarrow} \nu(\varepsilon)
$$

## Extension: Metric Spaces

Fact: In this framework, most of the results from this section still hold. We just need to replace $\nu$ by $\nu_{\delta}$.

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Future work: Can Turing's formula and concentration inequalities be extended to this framework?

