

Lecture 7

Small probs

Q1: Tue 2/4
beginning of class ≤ 15 min
All material up to
Small probs
L 1-8

→ LIII posted = ^{Lecture}notes
Resources websites
Notes → Figures from LIII

Lecture Notes III: Discrete probability in practice – Small Probabilities

Marina Meilă
mmp@stat.washington.edu

Department of Statistics
University of Washington

January, 2025

No chapter in Book

The problem with estimating small probabilities ←

by ML

Definitions and setup ←

Additive methods (Laplace, Dirichlet, Bayesian, ELE) ← why NOT

Discounting (Ney-Essen) ←

Multiplicative smoothing: Estimating the next outcome (Witten-Bell, Good Turing) ←
....

Back-off or shrinkage – mixing with simpler models

extra notes = pages not
used in the lecture

Data histogram, $n=15000$ samples from distribution over $m=9933$ chars

Summary of today's lecture

Methods

- Lap +1
- Bay +0.1 or smaller
- NE Ney - Essen
- WB Witten - Bell
- GT ϕ Good Turing
- GT 1 — " — variation

Rule 1: $n_j = n_{j'}$ $\Rightarrow \tilde{\theta}_j = \tilde{\theta}_{j'}$
for any method

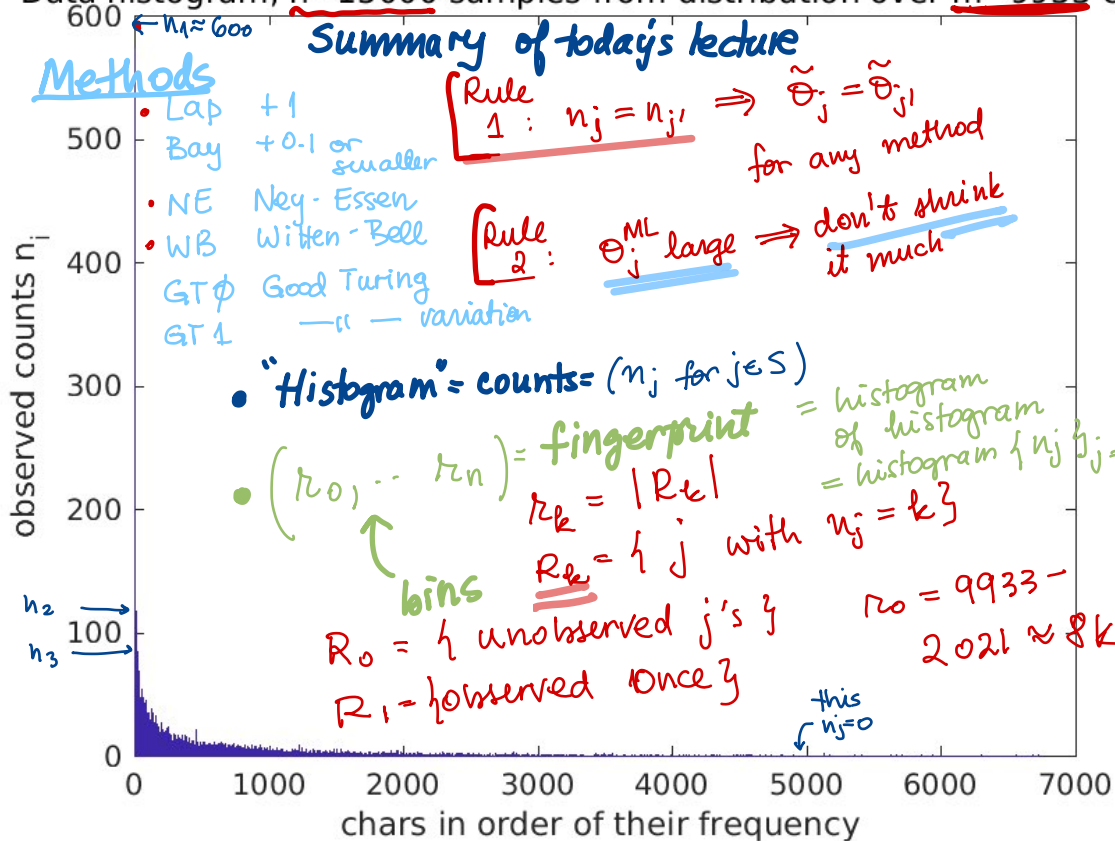
Rule 2: θ_j^{ML} large \Rightarrow don't shrink it much

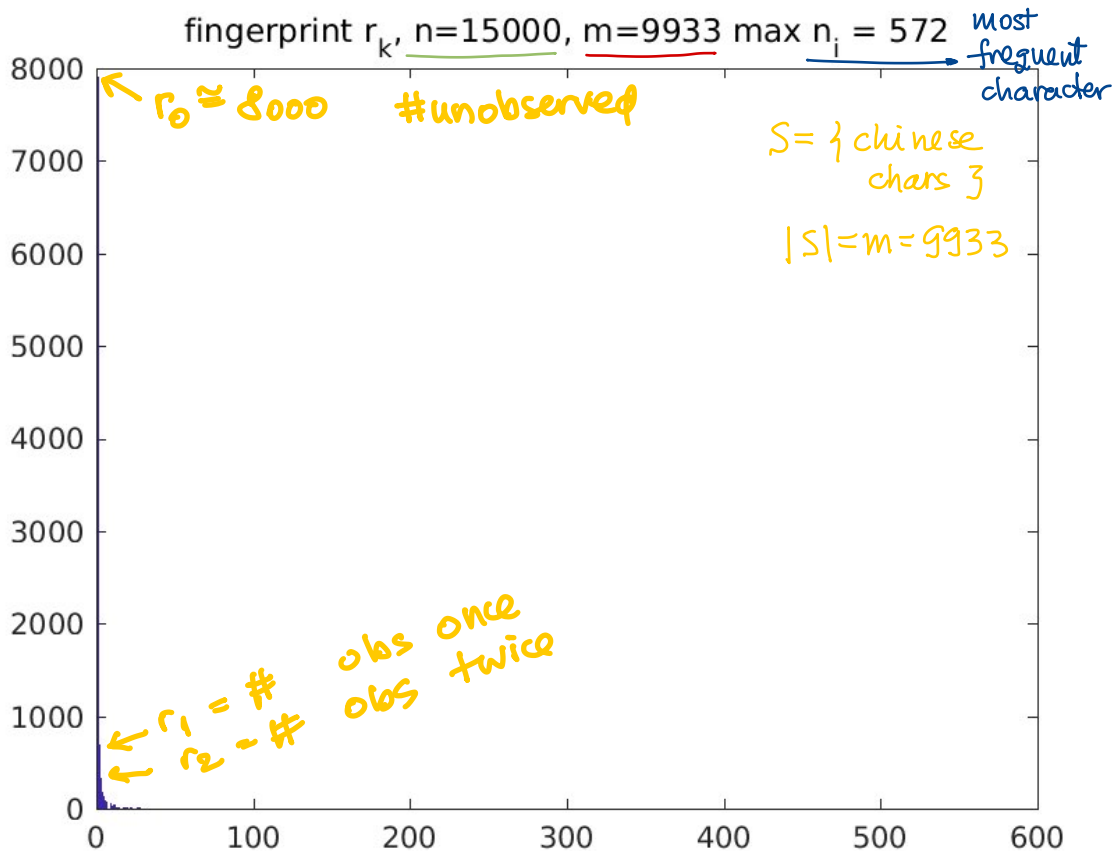
• "Histogram" = counts = $(n_j \text{ for } j \in S)$

• $(r_0, \dots, r_n) = \text{fingerprint}$
 $r_k = |R_k|$
 $R_k = \{j \text{ with } n_j = k\}$
 $r_0 = 9933 - 2021 \approx 8k$

$R_0 = \{ \text{unobserved } j \text{'s} \}$
 $R_1 = \{ \text{observed once} \}$

this $n_j=0$





Definitions and setup

extra notes

We will look at estimating categorical distributions from samples, when the number of outcomes m is large.

- ▶ Let $S = \{1, \dots, m\}$ be the sample space, and $P = (\theta_1, \dots, \theta_m)$ a distribution over S .
- ▶ We draw n independent samples from P , obtaining the **data set** \mathcal{D}
- ▶ Define the **counts** $\{n_j = \#j \text{ appears in } \mathcal{D}, i = 1, \dots, n\}$. The counts are also called **sufficient statistics** or **histogram**.
- ▶ Define the **fingerprint** (or **histogram of histogram**) of \mathcal{D} as the counts of the counts, i.e. $\{r_k = \# \text{counts } n_j = k, \text{ for } k = 0, 1, 2, \dots\}$

Example $m = 26$ alphabet letters

Data

the red fox is quick
 $n = 16$ letters

ho ho who s on first
 $n = 15$ letters

Counts n_j

$n_j = 0$: a, b, g, j, l, m, n,

p, v, w, y, z

$n_j = 1$: c, d, f, h, k, o, q, r, s, t, u, x

$n_j = 2$: e, i

$n_j = 0$: a, b, c, ..., x, z

$n_j = 1$: f, i, n, r, t, w

$n_j = 2$: s

$n_j = 3$: h

$n_j = 4$: o

Fingerprint r_k

$r_0 = 12 = |\{a, b, g, \dots, y, z\}|$

$r_1 = 12 = |\{c, d, f, h, \dots, u, x\}|$

$r_2 = 2 = |\{e, i\}|$

$r_3 = \dots r_n = 0$

$r_0 = 26 - 6 - 1 - 1 - 1 = 17$

$r_1 = 6 = |\{f, i, n, r, t, w\}|$

$r_2 = 1 = |\{s\}|$

$r_3 = 1 = |\{h\}|$

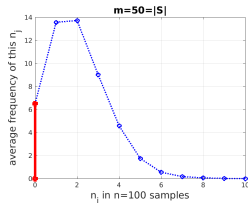
$r_4 = 1 = |\{o\}|$

- ▶ It is easy to verify that $n_j \in 0 : n$, hence $r_{0:n}$ may be non-zero (but $r_{n+1, n+2, \dots} = 0$), and that

$$m = r_0 + r_1 + \dots r_n \quad n = 0 \times r_0 + 1 \times r_1 + \dots k \times r_k + \dots \quad (1)$$

The problem with small probabilities and large m

extra notes



- ▶ when θ_i is small n must be very large to be able to observe i w.h.p.
- ▶ when m is large most θ_i are small
- ▶ Hence, in a sample of size n , many outcomes j may have $n_j = 0$, that is will not appear at all.
- ▶ **type k** $R_k = \{j \in S, n_j = k\}$ is the subset of outcomes in S that appear k times in \mathcal{D}
- ▶ Why are types important?
 - ▶ Because $\theta_j^{ML} = n_j/n$, all $i \in$ type k will have the same estimated value $\theta_j^{ML} = k/n$.
 - ▶ If $j, j' \in R_k$, no matter what correction method you use, there is no reason to distinguish between θ_j and $\theta_{j'}$. Hence $\theta_j = \theta_{j'}$ whenever $j, j' \in R_k$
 - ▶ Let $p_k = Pr[R_k]$. We have $p_k = r_k \theta_j$ for any $j \in R_k$.

The problem with estimating small probabilities

$$S = \{1, \dots, m\}$$

n samples

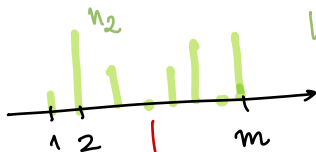
counts =
suff statistics

$$\begin{aligned} n_1 &= \#\{x^i = 1\} \\ n_j &= \# j \\ &\vdots \\ n_m &= \# m \end{aligned}$$

$$n_j \geq 0$$

$$\sum_{j=1}^m n_j = n$$

Want $\theta_{1:j} = P_r[j]$
 $j \in S$



1. $\theta_j^{ML} = \frac{n_j}{n}$

2. Smooth $\theta_{1:m}^{ML} \rightarrow \tilde{\theta}_{1:m}$

$n_j = 0 \Rightarrow \theta_j^{ML} = 0$

**NOT
ACCEP
TABLE
!!!**

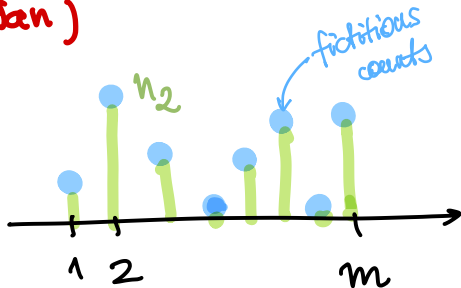
The problem with estimating small probabilities

Laplace (Bayesian)

1. $\tilde{n}_j = 1 + n_j$

$0.1 \rightarrow \tilde{n} = n + \frac{m}{10}$

fictitious samples



total = m ———

$$\tilde{n} = \sum_{j=1}^m \tilde{n}_j = \underline{n} + \underline{m}$$

2. $\tilde{\theta}_j^L = \frac{\tilde{n}_j}{\tilde{n}} = \frac{n_j + 1}{n + m}$

Shrinks
too much!!

!!!

$$\tilde{\theta}_1 = \frac{101}{150} = 0.67$$

$$\tilde{\theta}_{2:50} = \frac{1}{150}$$

Starting the car

Ex: $n = 100$

$m = 50$ possible outcomes

$$n_1 = 100$$

$$n_{2:50} = 0$$

$$\tilde{n} = 100 + 50 = 150$$

$$\tilde{n}_1 = 101$$

$$\tilde{n}_{2:50} = 1$$

The problem with estimating small probabilities

$$S = \{ \text{red wood, cherry, oak, acacia} \} \quad m=4$$
$$n=100$$

$$n_1 = 33 \quad +1$$

$$n_2 = 33 \quad +1$$

$$n_{\text{oak}} = 34 \quad +1$$

$$n_a = 0 \quad +1$$

Smoothing on an example

- ▶ the counts $\{n_j = \#j \text{ appears in } \mathcal{D}, i = 1, \dots, n\}$ (or **sufficient statistics** or **histogram**)
- ▶ **fingerprint** (or **histogram of histogram**) of \mathcal{D} as the counts of the counts $\{r_k = \# \text{counts } n_j = k, \text{ for } k = 0, 1, 2, \dots\}$, and $R_k = \{j, n_j = k, \}$

Example $m = 26$ alphabet letters

Data

data
↳

the red fox is quick
 $n = 16$ letters

Counts n_j

$n_j=0$: a, b, g, j, l, m, n,

p, v, w, y, z

$n_j=1$: c, d, f, h, k, o, q, r, s, t, u, x

$n_j=2$: e, i

Fingerprint r_k

$r_0 = 12 = |\{a, b, g, \dots, y, z\}|$

$r_1 = 12 = |\{c, d, f, h, \dots, u, x\}|$

$r_2 = 2 = |\{e, i\}|$ R_2

$r_3 = \dots r_n = 0$

$$r_1 = 12$$

$$r_2 = 2$$

$$n = 2 \cdot r_2 + 1 \cdot r_1 = 16$$

$$n = \sum_{j=1}^m n_j = 0 \cdot r_0 + 1 \cdot r_1 + 2 \cdot r_2 + \dots$$

$$= \sum_{k=0}^n k r_k$$

$$n = 14$$

For all k : $R_k = \{ \text{letters appear } k \text{ times} \} = \{j, n_j = k\}$

↳ $\tilde{\theta}_j$ the same for all $j \in R_k$

$$r = m - r_0 =$$

$$= \# \text{outcomes observed}$$

Smoothing on an example

ML, Lap, NeyEssen

- ▶ the counts $\{n_j = \#j \text{ appears in } \mathcal{D}, i = 1, \dots, n\}$ (or **sufficient statistics** or **histogram**)
- ▶ **fingerprint** (or **histogram of histogram**) of \mathcal{D} as the counts of the counts $\{r_k = \# \text{counts } n_j = k, \text{ for } k = 0, 1, 2, \dots\}$, and $R_k = \{j, n_j = k\}$

Example $m = 26$ alphabet letters

Data

the red fox is quick
 $n = 16$ letters

Counts n_j

$n_j = 0: a, b, g, j, l, m, n,$

p, v, w, y, z

$n_j = 1: c, d, f, h, k, o, q, r, s, t, u, x$

$n_j = 2: e, i$

Fingerprint r_k

$r_0 = 12 = |\{a, b, g, \dots, y, z\}|$

$r_1 = 12 = |\{c, d, f, h, \dots, u, x\}|$

$r_2 = 2 = |\{e, i\}|$

$r_3 = \dots r_n = 0$

$$ML: \theta_{a,b,g}^{ML} = 0 \quad \theta_{c,d}^{ML} = \frac{1}{16} \quad \theta_{e,i}^{ML} = \frac{2}{16} \quad \tilde{n} = n + m = 26 + 16 = 42$$

$$Lap: \tilde{\theta}_{a,b,g,\dots}^L = \frac{1}{42} \quad \tilde{\theta}_{c,d,\dots}^L = \frac{2}{42} \quad \tilde{\theta}_{e,i}^L = \frac{3}{42} \quad \frac{r_k}{m} = \frac{14}{26}$$

NeyEssen: Tax & redistribute
NE 1. Tax

$$n_j \geq 1 \Rightarrow n'_j = n_j - 1 \Rightarrow T = 12$$

$$n_j = 0 \Rightarrow n'_j = 0$$

2. Red

$$\tilde{n}_j = n'_j + \frac{T}{m} = n'_j + \frac{12}{m}$$

Rem: $n_j \notin \{1, 0\} \Rightarrow \tilde{\theta}_j$ same • n_j larger $\frac{n_j - 1}{n_j} \rightarrow 1$

$$\tilde{\theta}^{NE} = \begin{cases} 7/13 & n_j = 0 \\ 7/13 & n_j = 1 \\ 20/13 & n_j = 2 \end{cases}$$

Smoothing on an example

- ▶ the counts $\{n_j = \#j \text{ appears in } \mathcal{D}, i = 1, \dots, n\}$ (or **sufficient statistics** or **histogram**)
- ▶ **fingerprint** (or **histogram of histogram**) of \mathcal{D} as the counts of the counts $\{r_k = \# \text{counts } n_j = k, \text{ for } k = 0, 1, 2, \dots\}$, and $R_k = \{j, n_j = k\}$

$n = \# \text{observed outcomes}$

Example $m = 26$ alphabet letters

Data

the red fox is quick
 $n = 16$ letters

Counts n_j

$n_j = 0$: a, b, g, j, l, m, n,

p, v, w, y, z

$n_j = 1$: c, d, f, h, k, o, q, r, s, t, u, x

$n_j = 2$: e, i

Fingerprint r_k

$r_0 = 12 = |\{a, b, g, \dots, y, z\}|$

$r_1 = 12 = |\{c, d, f, h, \dots, u, x\}|$

$r_2 = 2 = |\{e, i\}|$

$r_3 = \dots r_n = 0$

NE

1. Tax

$$n_j \geq 1 \Rightarrow n'_j = n_j - 1 \Rightarrow \underline{T = n} = \text{total tax}$$

2. Red

$$\tilde{n}_j = n'_j + \frac{T}{m} = n'_j + \frac{n}{m}$$

1) n large $n \approx m \Rightarrow T \approx m \Rightarrow \frac{n}{m} \approx 1 = \tilde{n}_j \quad j \in R_0 \cup R_1$

2) n small $n \approx m \Rightarrow \frac{n}{m} = \delta \ll 1 \Rightarrow \text{for } j \in R_0 \cup R_1$

$$\tilde{n}_j = \frac{\delta}{n_0} = \frac{n}{n_0 m}$$

small!

Witten-Bell discounting – probability of a new value

NE
 R_0, R_1, R_2, \dots
 WB

$y = \begin{cases} 0 & \text{old} \\ 1 & \text{new letter} \end{cases}$

Ex the quicker fox is
 $\#y=1 = r$
 $\#y=0 = n-r$

► Idea:

- Look at the sequence (x_1, \dots, x_n) as a binary process: either we observe a value of X that was observed before, or we observe a new one.
- Assume that of m possible values r were observed (and $m - r$ unobserved)
- Then the probability of observing a new value is $p_0 = \frac{r}{n}$.
- Hence, set the probability of all unseen values of X to p_0 . The other probability estimates are renormalized accordingly.

$$\theta_j^{WB} = \begin{cases} \frac{n_j}{n} \frac{1}{1+p_0} = \frac{n_j}{n+r} & n_j > 0 \\ \frac{1}{m-r} \frac{p_0}{1+p_0} = \frac{1}{m-r} \frac{r}{n+r} & n_j = 0 \end{cases} \quad (7)$$

Witten-Bell makes sense only when some n_j counts are zero. If all $n_j > 0$ then W-B smoothing has undefined results.

WB smoothing has no parameter to choose (GOOD!)

Additive methods (Laplace)

extra notes

- **Idea:** assume we have seen one more example of each value in S
- **Algorithm:** add 1 to each count and renormalize.

$$\theta_j^{Laplace} = \frac{n_j + 1}{n + m} \quad \text{for } j = 1 : m \quad (2)$$

- Can be used also with another value, $n_j^0 < 1$, in place of 1.

Then, it is called **Bayesian mean smoothing** or **Dirichlet smothing** or **ELE**¹

Can be derived from Bayesian estimation, with the **Dirichlet prior**. In particular, we can take $n^0 = 1$, $n_j^0 = \frac{1}{m}$.

$$\theta_j^{Bayes} = \frac{n_j + n_j^0}{n + n_0} \quad \text{for } j = 1 : m \quad (3)$$

The “fictitious sample size” $n^0 = \sum_{j=1}^m n_j^0$ reflects the strength of our belief about the θ_j 's; if we choose all $n_j \propto \frac{1}{m}$, we say that we have an *uninformative prior*,

¹In natural language processing.

Problems with additive smoothing

extra notes

- ▶ Reduces all estimates **in the same proportion**
- ▶ Does not distinguish between spread and concentrated distributions.
 - ▶ the unseen outcomes have the same probability no matter how the counts are distributed
- ▶
- ▶ “Naive” method – DON'T USE IT

Ney-Essen discounting – tax and redistribute

extra notes

- Let r = the number of distinct values observed

$$r = m - r_0$$

► **Idea**

Tax subtract 1 observation from every $n_j > 0$

- i.e from each n_j that “can afford it”
- total amount = r

Red redistribute the total amount equally to **all** counts.

This simple method works surprisingly well in practice.

► **Algorithm**

$$r = \sum_{j=1:m} \min(n_j, 1) \quad \text{total tax collected} \quad (4)$$

$$n_j^{NE} = \max(n_j - 1, 0) + r/m \quad \text{redistribute} \quad (5)$$

$$\theta_j^{NE} = \frac{n_j^{NE}}{n} \quad \text{estimate from new counts} \quad (6)$$

Algorithm can be generalized to any “tax amount” $\delta > 0$.

- Then, the total tax collected is $D = \sum_j \min(n_j, \delta)$
- The smoothed counts are $n_j^{NE} = \max(n_j - \delta, 0) + D/m$

Properties of NE smoothing

extra notes

Flexibility

- ▶ treats outcomes with $n_j = 1$ and $n_j = 0$ the same

Intuition: any outcome i with $n_j < \delta$ is a rare outcome and should be treated in the same way, no matter how many observations it actually has.

- ▶ For m large and r small
 - ▶ (probability mass is concentrated on a few values)
 - ▶ r small \Rightarrow unobserved outcomes receive little probability
- ▶ For m large and r large
 - ▶ $r \approx m$ (large) \Rightarrow unobserved outcomes get $n^{NE} \approx 1$
- ▶ For tax $\delta \neq 1$, note $D \leq \delta r$, redistributed mass $\frac{D}{m} \leq \delta \frac{r}{m}$

Witten-Bell discounting – probability of a new value

extra notes

► Idea:

- Look at the sequence (x_1, \dots, x_n) as a binary process: either we observe a value of X that was observed before, or we observe a new one.
- Assume that of m possible values r were observed (and $m - r$ unobserved)
- Then the probability of observing a new value is $p_0 = \frac{r}{n}$.
- Hence, set the probability of all unseen values of X to p_0 . The other probability estimates are renormalized accordingly.

$$\theta_j^{WB} = \begin{cases} \frac{n_j}{n} \frac{1}{1+p_0} = \frac{n_j}{n+r} & n_j > 0 \\ \frac{1}{m-r} \frac{p_0}{1+p_0} = \frac{1}{m-r} \frac{r}{n+r} & n_j = 0 \end{cases} \quad (7)$$

Witten-Bell makes sense only when some n_j counts are zero. If all $n_j > 0$ then W-B smoothing has undefined results.

WB smoothing has no parameter to choose (GOOD!)

Good-Turing – Predicting the type of the next outcome extra notes

- ▶ This method has many versions (you will see why). Powerful for large data sets.

▶ First Idea

- ▶ Remember $r_k = \#\{j, n_j = k\}$ the counts of the counts. Naturally, $n = \sum_{k=1}^{\infty} k r_k$.
- ▶ Outcome i is of type k if $n_j = k$. GT uses the data to estimate the probability of type k

$$p_k = \frac{k r_k}{n} \quad \text{for } k = 1 : n \quad (8)$$

- ▶ Second Idea is to use the probabilities $p_1, \dots, p_k \dots$ to predict the next outcome

- ▶ For example, what's the probability of seeing a new value?
It must be equal to p_1 , because this observation will have count $n_j = 1$ once it is observed.
- ▶ Similarly, the probability of observing a type k outcome must be about p_{k+1} .

- ▶ Third There are r_k outcomes j in type k , hence the probability mass for each of these is $1/r_k$ of p_{k+1} which leads to (11).

▶ Algorithm

$$\text{if } n_j = k \quad \theta_j^{GT} = \frac{p_{k+1}}{r_k} = \frac{(k+1)r_{k+1}}{n r_k} \stackrel{\text{def}}{=} \frac{n_k^{GT}}{n} \quad \text{with} \quad n_j^{GT} = \frac{(k+1)r_{k+1}}{r_k} \quad (9)$$

In particular if $n_j = 0$

$$\theta_j^{GT} = \frac{p_1}{r_0} \quad (10)$$

- ▶ Remark GT transfers the probability mass of type $k+1$ to type k
- ▶ This implies that

$$n_j^{GT} r_k = (k+1)r_{k+1} \text{ if } n_j = k \quad (11)$$

Problems with Good-Turing

extra notes

- ▶ When k is large, r_k is small and noisy.
 - ▶ **Example** The word “Jimmy” appears $n_{Jimmy} = 8196$ times in a corpus. But there may be no word that appears 8197 times. Then, $\theta_{Jimmy}^{GT} = 0!$
- ▶ Remedy: “smooth” the r_k values, i.e use (an estimate of) $E[r_k]$
 - ▶ Many proposals exist
 - ▶ A simple one is to use Good-Turing only for type 0, and to rescale the other θ^{ML} estimates down to ensure normalization.

$$\theta_j^{GT} = \begin{cases} \frac{p_1}{r_0} = \frac{r_1}{nr_0} & \text{if } n_j = 0 \\ \theta_j^{ML} \left(1 - \frac{r_1}{n}\right) & \text{if } n_j > 0 \end{cases} \quad (12)$$

Comparison of the methods

extra notes

Numerical values to exemplify the results: $n = 1000$, $m = 1000$, $r = 100$

Count n_j	0	1	$n_j \gg 1$
θ_j^{ML}	0	$\frac{1}{n} = \frac{1}{1000}$	$\frac{n_j}{1000}$
$\theta_j^{Laplace}$	$\frac{1}{n+m} = \frac{1}{2000}$	$\frac{2}{n+m} = \frac{1}{1000}$	$\frac{n_j+1}{n+m} = \frac{n_j+1}{2000}$
θ_j^{Bayes} , $n^0 = 1$, $n_j^0 = \frac{1}{m}$	$\frac{1}{m(n+1)} \approx \frac{1}{10^6}$	$\frac{1+1/m}{n+1} \approx \frac{1}{10^3}$	$\frac{n_j+1/m}{n+1} \approx \frac{n_j}{1000}$
θ_j^{NE} , $\delta = 1$	$\frac{r}{mn} = \frac{1}{10^4}$	$\frac{r}{mn} = \frac{1}{10^4}$	$\frac{n_j-1+r/m}{n} \approx \frac{n_j}{1000}$
θ_j^{WB}	$\frac{1}{m-r} \frac{r}{n+r} = \frac{1}{9900}$	$\frac{1}{n+r} = \frac{1}{1100}$	$\frac{n_j}{n+r} = \frac{n_j}{1100}$

Remarks

- ▶ Laplace shrinks ML estimates of large probabilities by factor of 2. **Too much!** (because large θ_j^{ML} are close to their true values)
- ▶ Bayes (with uninformative prior) affects large θ_j^{ML} much less than small ones. **Good**
- ▶ Ney-Essen smooths more when r is larger; any n_j is affected by less than δ .
- ▶ Ney-Essen estimates of θ^{NE} for counts of 0 and 1 are equal to a fraction of $\frac{r}{m}$ (this grows with n as r grows with n).
- ▶ In Witten-Bell, the large θ_j^{ML} are shrunk depending on r , but independently of m . **Proportional, bad**
- ▶ ... but, if we overestimate m grossly, the overestimation will only affect the θ_j^{WB} for the 0 counts, but none of the θ_j^{WB} for the values observed. (true for NE as well).