# An Introduction to Heavy Tails for ML Researchers

Conspiracies, Catastrophes, and the Principle of a Single Big Jump

Adam Wierman, Caltech

# An Introduction to Heavy Tails for ML Researchers

Conspiracies, Catastrophes, and the Principle of a Single Big Jump

### Material based on:



"The top 1% of a population owns 40% of the wealth; the top 2% of Twitter users send 60% of the tweets. These figures are always reported as shocking [...] as if anything but a bell curve were an aberration, but Pareto distributions pop up all over. Regarding them as anomalies prevents us from thinking clearly about the world."

- Clay Shirky in Newsweek (2011)

"The top 1% of a population owns 40% of the wealth; the top 2% of Twitter users send 60% of the tweets. These figures are always reported as shocking [...] as if anything but a bell curve were an aberration, but Pareto distributions pop up all over. Regarding them as anomalies prevents is from thinking clearly about the world." ML researchers

- Clay Shirky in Newsweek (2011)





# In ML/AI, heavy tails are common in inputs to models & created by core algorithms like SGD.

10:30 - 11:10	Invited talk: Liam Hodgkinson	Overparameterization and the Power Law Paradigm
11:10 - 11:35	Contributed talk: Vivien Cabannes	Associative Memories with Heavy-Tailed Data
11:35 - 12:00	Contributed talk: Dominique Perrault-Joncas	Meta-Analysis of Randomized Experiments
12:00 - 14:00 14:00 - 14:40 14:40 - 15:05	Invited talk: Nisha Chandramoorthy Contributed talk: Jeremy Cohen	A dynamical View of Learners, Samplers and Forecasters Adaptive Gradient Methods at the Edge of Stability
15:05 - 15:30	Coffee break	
15:30 - 16:10	Invited talk: Charles Martin	Heavy-Tailed Self -Self-Regularization in DNNs

In ML/AI, heavy tails are common in inputs to models & created by core algorithms like SGD.

...yet many ML algorithms are designed and analyzed using intuition and tools based on light-tailed assumptions.

Heavy-tailed phenomena are typically treated as something



Our intuition is flawed because intro probability classes treat heavy-tails as curiosities

Simple, appealing statistical approaches for estimating them have BIG problems

# <u>An historic example:</u> Networking "discovers" heavy tails (early 2000s)



The existence of heavy-tails required rethinking network design & communication protocols











# What order should jobs be served in to minimize Pr(Delay > t) for large t?

 Home > Operations Research > Vol. 60, No. 5 >

 Is Tail-Optimal Scheduling Possible?

 Adam Wierman, Bert Zwart

 Published Online: 9 Oct 2012 | https://doi.org/10.1287/opre.1120.1086

### Example: The fragility of the internet



### Example: The fragility of the internet



But all was not as it seemed...



social networks, biology, astronomy, chemistry,...

### Many of the controversies are still not resolved...

Scale-free networks are rare Anna D. Broido<sup>1,\*</sup> and Aaron Clauset<sup>2,3,4,†</sup> <sup>1</sup>Department of Applied Mathematics, University of Colorado, Boulder, CO, USA <sup>2</sup>Department of Computer Science, University of Colorado, Boulder, CO, USA <sup>3</sup>BioFrontiers Institute, University of Cd <sup>4</sup>Santa Fe Institute, Santa A central claim in modern network science is that remeaning that the fraction of nodes with degree k follow  $2 < \alpha < 3$ . However, empirical evidence for this beli Ivan Voitalov,<sup>1,2</sup> Pim van der Hoorn,<sup>1,2</sup> Remco van der Hofstad,<sup>3</sup> and Dmitri Krioukov<sup>1,2,4,5</sup> real-world networks. We test the universality of scal statistical tools to a large corpus of nearly 1000 net technological, and informational sources. We fit the test its statistical plausibility, and compare it via a free models, e.g., the log-normal. Across domains, only 4% exhibiting the strongest-possible evidence weakest-possible evidence. Furthermore, evidence of across sources: social networks are at best weakly biological networks can be called strongly scale fr scale-free networks and reveal that real-world net likely require new ideas and mechanisms to expla

### Scale-Free Networks Well Done

<sup>1</sup>Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA <sup>2</sup>Network Science Institute, Northeastern University, Boston, Massachusetts 02115, USA <sup>3</sup>Department of Mathematics and Computer Science, Eindhoven University of Technology, Postbus 513, 5600 MB Eindhoven, Netherlands

<sup>4</sup>Department of Mathematics, Northeastern University, Boston, Massachusetts 02115, USA <sup>5</sup>Department of Electrical & Computer Engineering, Northeastern University, Boston, Massachusetts 02115, USA

We bring rigor to the vibrant activity of detecting power laws in empirical degree distributions in real-world networks. We first provide a rigorous definition of power-law distributions, equivalent to the definition of regularly varying distributions that are widely used in statistics and other fields. This definition allows the distribution to deviate from a pure power law arbitrarily but without affecting the power-law tail exponent. We then identify three estimators of these exponents that are proven to be statistically consistent—that is, converging to the true value of the exponent for any regularly varying distribution—and that satisfy some additional niceness requirements. In contrast to estimators that are currently popular in network science, the estimators considered here are based on fundamental results in extreme value theory, and so are the proofs of their consistency. Finally, we apply these estimators to a representative collection of synthetic and real-world data. According to their estimates, real-world scale-free networks are definitely not as rare as one would conclude based on the popular but unrealistic assumption that real-world data comes from power laws of

### All of this has happened before. All of this will happen again.

- Battlestar Galactica (orig. from Peter Pan by J.M. Barrie)

#### Isaac Newton Institute for Mathematical Sciences

### 15 December 2023 – Rooms R02-R05 – New Orleans Convention Center Heavy Tails in ML Heavy tails in Structure, Stab ML/Al is next! Home > What's On > Programmes & Workshops Heavy tails in machine learning

a NeurIPS 2023 Workshop

Dynamics

Heavy-tails and chaotic behavior naturally appear in many ways in We aim to create an environment to study how they emerge and how th

#### Description

Heavy-tailed distributions likely produce observations that can be very and far from the mean; hence, they are often used for modeling pheno outliers. As a consequence, the machine learning and statistics comm heavy-tailed behaviors with rather negative consequences, such as c

0

Heavy-Tails-ML-2023

#### Programme theme

HEAVY TAILS IN MACHINE LEARNING

The Stochastic Gradient Descent (SGD) algorithm is both fundamental and ubiquitous in Machine Learning applications. In recent years, heavy-tailed distributions have been observed in practice implementations of the SGD algorithm. Importantly, the heavy-tailed behaviour is generally not a consequence of the presence of a heavy-tailed distribution in the description of the model. It is not understood under what circumstances heavy tails arise in SGD and, when they do, what their effects on the performance of the SGD

The INI satellite programme at the Alan Turing Institute will initiate a research programme centered around the following questions:

- When and how do heavy-tailed phenomena arise in general SGD
- How should the SGD algorithm be modified to make it efficient in the

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#### Organisers

- O. Deniz Akyildiz Imperial College
- Anita Behme Technische Universität Dresden
- Emilie Chouzenoux Université Paris Saclay
- Jorge Gonzalez-Cazares University of Warwick; The Alan Turing Institute
- Aleksandar Mijatovic University of Warwick; The Alan Turing Institute

#### Participants

O. Deniz Akyildiz Imperial College

Heavy-tailed phenomena are typically treated as something



Our intuition is flawed because intro probability classes focus on light-tailed distributions

approaches for estimating them have BIG problems





Canonical Example: The Pareto Distribution a.k.a. the "power-law" distribution  

$$Pr(X > x) = \overline{F}(x) = \left(\frac{x_{\min}}{x}\right)^{\alpha}$$
 for  $x \ge x_{\min}$   
p.d.f:  $f(x) = \frac{\alpha x_{\min}^{\alpha}}{x^{\alpha+1}}$ 

Notice:  $Var[X] = \infty$  if  $\alpha < 2!$ 

<u>Canonical Example</u>: The Pareto Distribution a.k.a. the "power-law" distribution <u>Many other examples</u>: LogNormal, Weibull, Zipf, Cauchy, Student's t, Frechet, ... <u>Canonical Example</u>: The Pareto Distribution a.k.a. the "power-law" distribution

Many other examples: LogNormal, Weibull, Zipf, Cauchy, Student's t, Frechet, ...

X: 
$$\log X \sim Normal$$
  
 $Var[X] = (e^{\sigma^2} - 1)e^{2\mu + \sigma^2}$ 

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<u>Many other examples</u>: LogNormal, Weibull, Zipf, Cauchy, Student's t, Frechet, ...

$$\bar{F}(x) = e^{-(x/\lambda)^k}$$

k < 1: Heavy – tailed k = 1: Exponential k = 3.4: Approx Normal  $k \rightarrow \infty$ : Deterministic

# Heavy-tailed distributions have many strange & beautiful properties

- The "Pareto principle" (e.g. 80% of the wealth owned by 20% of the population)
- Infinite variance or even infinite mean
- Outliers that are much larger than the mean happen "frequently"

# These are driven by 3 "defining" properties

- 1) Scale invariance
- 2) The "catastrophe principle"
- 3) The residual life "blows up" (see the book!)





# Scale invariance

*F* is scale invariant if there exists an  $x_0$  and a *g* such that  $\overline{F}(\lambda x) = g(\lambda)\overline{F}(x)$  for all  $\lambda$ , *x* such that  $\lambda x \ge x_0$ .



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<u>Theorem</u>: A distribution is scale invariant if and only if it is Pareto.

**Example:** Pareto distributions

$$\overline{F}(\lambda x) = \left(\frac{x_{\min}}{\lambda x}\right)^{\alpha} = \overline{F}(x) \left(\frac{1}{\lambda}\right)^{\alpha}$$

# Scale invariance

*F* is scale invariant if there exists an  $x_0$  and a *g* such that  $\overline{F}(\lambda x) = g(\lambda)\overline{F}(x)$  for all  $\lambda$ , *x* such that  $\lambda x \ge x_0$ .



# Asymptotic scale invariance

 $F \text{ is asymptotically scale invariant if there exists a continuous, finite } g \text{ such that} \\ \lim_{x \to \infty} \frac{\bar{F}(\lambda x)}{\bar{F}(x)} = g(\lambda) \text{ for all } \lambda.$ 

### **Example:** Regularly varying distributions

*F* is regularly varying if  $\overline{F}(x) = x^{-\rho}L(x)$ , where L(x) is slowly varying, i.e.,  $\lim_{x \to \infty} \frac{L(xy)}{L(x)} = 1$  for all y > 0.

<u>Theorem</u>: A distribution is asymptotically scale invariant iff it is regularly varying.

# Asymptotic scale invariance

 $F \text{ is asymptotically scale invariant if there exists a continuous, finite } g \text{ such that} \\ \lim_{x \to \infty} \frac{\bar{F}(\lambda x)}{\bar{F}(x)} = g(\lambda) \text{ for all } \lambda.$ 

### **Example:** Regularly varying distributions

*F* is regularly varying if  $\overline{F}(x) = x^{-\rho}L(x)$ , where L(x) is slowly varying, i.e.,  $\lim_{x \to \infty} \frac{L(xy)}{L(x)} = 1$  for all y > 0.

Regularly varying distributions are extremely easy to work with analytically. They behave like Pareto distributions with respect to the tail.

- → "Karamata" theorems
- $\rightarrow$  "Tauberian" theorems
### Heavy-tailed distributions have many strange & beautiful properties

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# A thought experiment

Suppose that during lecture I polled <u>50 students</u> about their heights and the number of instagram followers they have...

The sum of the heights was ~300 feet. The sum of the number of instagram followers was 1,025,000 What led to these large values?

# A thought experiment

Suppose that during lecture I polled <u>50 students</u> about their heights and the number of instagram followers they have...

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8'3" (2.5m)



614 million followers

# A thought experiment

Suppose that during lecture I polled <u>50 students</u> about their heights and the number of instagram followers they have...

The sum of the heights was ~300 feet. The sum of the number of instagram followers was 1,025,000

A bunch of people were probably just over 6' tall (Maybe the basketball teams were in the class.) *Conspiracy principle* 0

One person was probably a social media celebrity and had ~1 million followers. *Catastrophe principle* 

### Example

Consider  $X_1, X_2$  i.i.d. Weibull with mean 1. Given the rare event  $X_1 + X_2 = 10$ , what is the marginal density of  $X_1$ ?



### Example

Consider  $X_1, \ldots, X_{20}$  i.i.d. Weibull with mean 1. Given the rare event  $X_1 + \cdots + X_{20} = 200$ , what is the marginal density of  $X_1$ ?



"Catastrophe principle"  $Pr(max(X_1, ..., X_n) > t) \sim Pr(X_1 + \dots + X_n > t)$  $\Rightarrow \Pr(\max(X_1, \dots, X_n) > t | X_1 + \dots + X_n > t) \rightarrow 1$ 

"Conspiracy principle"  $Pr(\max(X_1, ..., X_n) > t) = o(Pr(X_1 + \dots + X_n > t))$ 



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### **Subexponential distributions**

F is subexponential if for i.i.d.  $X_i$ ,  $Pr(X_1 + \dots + X_n > t) \sim nPr(X_1 > t)$ 



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### Heavy-tailed distributions have many strange & beautiful properties

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# These are driven by 3 "defining" properties

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#### Where do heavy-tails come from in ML/AI applications?

<u>Option 1</u>. They come from the data (and costs) in the applications.

<u>Option 2</u>. They are created by the algorithms we use.

 $\min_{x\in\mathbb{R}}f(x)$ 

 $\min_{x\in\mathbb{R}} E[Ax^2 + Bx]$ 

Assuming E[A] > 0 and gradients are available, SGD with learning rate  $\eta$  follows

$$X_{k+1} = X_k - \eta (2A_k X_k + B_k)$$

 $\min_{x\in\mathbb{R}} E[Ax^2 + Bx]$ 

Assuming E[A] > 0 and gradients are available, SGD with learning rate  $\eta$  follows

$$X_{k+1} = \underbrace{X_k - \eta(2A_k X_k + B_k)}_{C_k}$$

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Assuming E[A] > 0 and gradients are available, SGD with learning rate  $\eta$  follows

 $X_{k+1} = C_k X_k + \eta B_k$ 

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$$\uparrow$$
$$D_k$$

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$$X_{k+1} = C_k X_k + D_k$$

This process is both *multiplicative* and *additive*.

### We know a lot about additive processes!

We've all been taught that the Gaussian is "normal" because of the Central limit theorem



But the Central Limit Theorem we're taught in intro probability is not complete!

Consider i.i.d.  $X_i$ . How does  $\sum_{i=1}^n X_i$  grow?

Law of Large Numbers (LLN):  $\frac{1}{n} \sum_{i=1}^{n} X_i \to E[X_i] \ a.s.$  when  $E[X_i] < \infty$ 

Consider i.i.d.  $X_i$ . How does  $\sum_{i=1}^n X_i$  grow?

Law of Large Numbers (LLN):  $\sum_{i=1}^{n} X_i = nE[X_i] + o(n)$ 



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Consider i.i.d.  $X_i$ . How does  $\sum_{i=1}^{n}$  What if  $Var[X_i] = \infty$ ? Law of Large Numbers (LLN):  $\sum_{i=1}^{n} X_i = nE[X_i] + o(n)$ Central Limit Theorem (CLT):  $\sum_{i=1}^{n} X_i = nE[X_i] + \sqrt{nZ}$ where  $Z \sim Normal(0, \sigma^2)$  with  $Var[X_i] = \sigma^2 < \infty$ .  $\prod_{i=1}^{n} X_i - nE[X_i]$  $\sum_{i=1}^{n} X_i$ 300 300 n n

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Law of Large Numbers (LLN):  $\sum_{i=1}^{n} X_i = nE[X_i] + o(n)$ Central Limit Theorem (CLT):  $\sum_{i=1}^{n} X_i = nE[X_i] + \sqrt{nZ} + o(\sqrt{n})$ 

where  $Z \sim Normal(0, \sigma^2)$  with  $Var[X_i] = \sigma^2 < \infty$ .



$$\sum_{i=1}^{n} X_i = nE$$
Finite variance  $\rightarrow$  Light-tailed (Normal)  
Infinite variance  $\rightarrow$  Heavy-tailed (power law) set

Additive processes can lead to heavy-tails, depending on the input.

What about multiplicative processes?

#### Multiplicative processes almost always lead to heavy tails

An example:

 $Y_{1}, Y_{2} \sim Exponential(\mu)$   $Pr(Y_{1} \cdot Y_{2} > x) \geq Pr(Y_{1} > \sqrt{x})^{2}$   $= e^{-2\mu\sqrt{x}}$  $\Rightarrow Y_{1} \cdot Y_{2} \text{ is heavy-tailed!}$ 



 $\min_{x\in\mathbb{R}} E[Ax^2 + Bx]$ 

Assuming E[A] > 0 and gradients are available, SGD with learning rate  $\eta$  follows

$$X_{k+1} = C_k X_k + D_k$$

This process is both *multiplicative* and *additive*.

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This process is both *multiplicative* and *additive*.

Under minor technical conditions,  $X_k \to F$  such that  $\lim_{x \to \infty} \frac{\log \overline{F}(x)}{\log x} = s^* \text{ where } s^* = \sup(s \ge 0 | E[X_k^s] \le 1)$ 

regularly varying  $\rightarrow$  SGD leads to heavy tails, even when A and B are light tailed!

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regularly varying  $\rightarrow$  <u>SGD leads to heavy tails, even when A and B are light tailed.</u> <u>& this leads to better generalization too!</u>



How does one "design" algorithms in the face of heavy tails?

Key: Minimize the impact of catastrophes





#### **Example:** Estimating the mean

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability:  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$
<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability:  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 



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#### Key: Minimize the impact of catastrophes

# Idea 1: Trim the outliers

[Tukey & McLaughlin 1963], [Bickel 1965], [Stigler 1973]

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

## Key: Minimize the impact of catastrophes

# Idea 1: Trim the outliers

1. Divide data into two equal parts. 2. Use first part to determine truncation points  $\beta = Y_{(1-\varepsilon)n}^*$  and  $\alpha = Y_{\varepsilon n}^*$ 3. Trim outliers using truncation points  $Y_i = [X_i]_{\alpha}^{\beta}$ 4. Estimate using sample mean of  $Y_i$ 

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

#### Key: Minimize the impact of catastrophes

#### Idea 1: Trim the outliers

$$\varepsilon(n,\delta) = 9\sigma \sqrt{\frac{\log 8/\delta}{n}}$$

+ it's robust to corruption! [Lugosi and Mendelson, 2019]

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

#### Key: Minimize the impact of catastrophes

#### Idea 1: Trim the outliers

# Idea 2: Median of means

[Nemirovsky and Yudin 1983], [Jerrum,Valiant, and Vazirani 1986], [Alon, Matias, and Szegedy 2002]

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

## Key: Minimize the impact of catastrophes

Idea 1: Trim the outliers

Idea 2: Median of means

Divide data into k equal groups.
Compute the sample average of each group.
Compute the median of the sample averages.

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

#### Key: Minimize the impact of catastrophes

Idea 1: Trim the outliers

Idea 2: Median of means

$$\varepsilon(n,\delta) = 9\sigma \sqrt{\frac{\log 8/\delta}{n}}$$

+ it works even when the variance is infinite! [Bubeck, Cesa-Bianchi, and Lugosi, 2013]

<u>Goal</u>: Given i.i.d. samples  $X_1, \ldots, X_n$  with mean  $\mu$ , develop estimates of the mean that are good with high probability,  $\Pr(|\hat{\mu}_n - \mu| > \varepsilon(n, \delta)) \leq \delta$ 

#### Key: Minimize the impact of catastrophes

Idea 1: Trim the outliers

Idea 2: Median of means

Note: Both methods depend on knowing  $\delta$  (when setting truncation/group sizes). This is unavoidable.









Heavy-tailed phenomena are typically treated as something



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#### For details, references, etc., see:

