

A study of systematic uncertainties within the MSHT PDF Framework

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Objectives

- Introduce a Model that can incorporate Error on Errors
- Examining how this model behaves for both uncorrelated and correlated systematic errors
- Investigate what this model tells us about 2 Data Sets ATLAS W,Z Data and ATLAS 7 TeV Inclusive Jet Distributions
- A brief investigation into de-correlation

Introduction

- Experimental data is becoming increasingly precise
- Experimental Errors are now dominated by systematic uncertainties
- Significant Errors on these systematic uncertainties
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- Significant Errors on these systematic uncertainties
- So we need to include these "errors on errors" to correctly determine the errors in PDF fits
- We need to depart from the simple Gaussian treatment of errors if we want to include these "Error on Errors"

Including Error on Errors 11

Gaussian

■ Consider a set of data, \mathbf{y} . The probability of \mathbf{y} can be written $P(\mathbf{y}|\mu,\theta)$, where μ are parameters of interest and θ are nuisance parameters that are required for the correctness of the model.

¹Cowan arXiv:1809.05778v3

Including Error on Errors 11

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- Let $\theta = (\theta_1, ..., \theta_N)$ be independent Gaussian distributed values $u = (u_1, ..., u_N)$, with standard deviations $\sigma_u = (\sigma_{u_1}, ..., \sigma_{u_N})$:

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$$L(\mu, \theta) = P(\mathbf{y}, \mathbf{u} | \mu, \theta) = P(\mathbf{y} | \mu, \theta) P(\mathbf{u} | \theta)$$

$$= P(\mathbf{y} | \mu, \theta) \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi} \sigma_{u_i}} e^{-(u_i - \theta_i)^2 / 2\sigma_{u_i}^2}$$
(1)

¹Cowan arXiv:1809.05778v3

Including Error on Errors 22

Gaussian plus Gamma

■ Model the estimated variances, v_i , of $\sigma_{u_i}^2$, as Gamma distributed gives:

$$L(\mu, \theta, \sigma_{u_i}^2) = P(y|\mu, \theta) \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i - \theta_i)^2/2\sigma_{u_i}^2} \frac{\beta_i^{\alpha_i}}{\Gamma(\alpha_i)} v_i^{\alpha_i - 1} e^{-\beta_i v_i}$$

$$\alpha_i = \frac{1}{4r_i^2} \qquad \beta_i = \frac{1}{4r_i^2 \sigma_{u_i}^2}$$

■ r_i is defined as the relative uncertainty in the estimate of the systematic error. The parameters r_i can therefore be referred to as the "error on errors".

²Cowan arXiv:1809.05778v3

Including Error on Errors 3

Gaussian plus Gamma = t-distribution

■ This model can be identically reinterpreted as a Student's t-distribution

$$L(\mu, \theta, \sigma_{u_i}^2) = P(y|\mu, \theta) \prod_{i=1}^{N} \frac{\Gamma(\frac{\nu_i + 1}{2})}{\sqrt{\nu_i \pi} \Gamma(\nu_i / 2)} \left(1 + \frac{t_i^2}{\nu_i} \right)^{-\frac{\nu_i + 1}{2}}$$
(2)

where
$$t_i = \frac{u_i - \theta_i}{\sqrt{v_i}}$$
 and $v_i = \frac{1}{2r_i^2}$.

■ So we can treat our nuisance parameters as t-distributed!

Consider the case:

$$y_i = d_i + errors = d_i + \sigma_i z_i + \sigma_{u_i} t_{u_i} + \sum_{j=1}^{M} \beta_{ij} t_j'$$
 (3)

where for each observable y_i we have

- One statistical error σ_i , with a z_i that is a Normally distributed fluctuating variable.
- One uncorrelated systematic error σ_{u_i} with a t_{u_i} that is a t-distributed fluctuating variable with dof of $\nu = 1/2r_{\chi^2}^2$
- M correlated systematic errors, β_{ij} , each with a fluctuation t'_j that are t-distributed with dof of $\nu = 1/2r_{\chi^2}^2$. These fluctuations are the same for all i.

Treating our z_i , t_{u_i} and t' as independent

■ The likelihood function can be written up to some constants as:

$$L \propto \prod_{i=1}^{N} \exp \left[-\frac{1}{2} \frac{(y_i - d_i - t_{u_i} \sigma_{u_i} - \sum_{j=1}^{M} \beta_{ij} t_j')}{\sigma_i^2} \right] \left(1 + \frac{t_{u_i}^2}{\nu} \right)^{-\frac{\nu+1}{2}} \times \prod_{j=1}^{M} \left(1 + \frac{t_j'^2}{\nu} \right)^{-\frac{\nu+1}{2}}$$
(4)

Naturally leading to the Loglikehihood equation:

$$\chi^{2} \equiv -2LnL = \sum_{i=1}^{N} \left(\frac{m_{i} - d_{i} - \sigma_{u_{i}} t_{u_{i}} - \sum_{j} \beta_{ij} t_{j}'}{\sigma_{j}} \right)^{2} + (\nu + 1) \sum_{i=1}^{N} Ln \left(1 + \frac{t_{u_{i}}^{2}}{\nu} \right) + (\nu + 1) \sum_{i=1}^{M} Ln \left(1 + \frac{t_{j}'^{2}}{\nu} \right)$$
 (5)

Treating our z_i , t_{u_i} and t' as independent (Cont.)

■ If we minimize with respect to t_{u_i} we obtain:

$$t_{u_{i}}^{3} \frac{\sigma_{u_{i}}^{2}}{\sigma_{i}^{2}} \frac{1}{\nu} - \frac{t_{u_{i}}^{2}}{\nu} (y_{i} - d_{i} - \sum_{j} \beta_{j} t_{j}^{\prime}) \frac{\sigma_{u_{i}}}{\sigma_{i}^{2}} + t_{u_{i}} \left(\frac{\sigma_{u_{i}}^{2}}{\sigma_{i}^{2}} + \frac{\nu + 1}{\nu} \right) - \frac{(y_{i} - d_{i} - \sum_{j} \beta_{j} t_{j}^{\prime}) \sigma_{u_{i}}}{\sigma_{i}^{2}} = 0$$

 \blacksquare Minimizing with respect to t_i' yields

$$\sum_{i=1}^{N} \frac{\beta_{ij}^{2}}{v\sigma_{i}^{2}} (t'_{j})^{3} + \frac{D}{v} (t'_{j})^{2} + \left(\left(\sum_{i=1}^{N} \frac{\beta_{ij}^{2}}{\sigma_{i}^{2}} \right) + \frac{v+1}{v} \right) t'_{j} + D = 0$$

$$D = -\sum_{i=1}^{N} \frac{(y_{i} - d_{i} - \sigma_{u_{i}} t_{u_{i}} - \sum_{j \neq j'}^{M} \beta_{ij} t'_{j}) \beta_{ij'}}{\sigma_{i}^{2}}.$$

■ Solved Simultaneously. t_{u_i} solved analytically, t'_i has to be fitted.

Behaviour as $r \rightarrow 0$

 \blacksquare As r o 0, $v o \infty$:

$$-2LnL = \sum_{i=1}^{N} \left(\frac{y_i - d_i - \sigma_{u_i} t_{u_i} - \sum_{j} \beta_{ij} t'_j}{\sigma_i} \right)^2 + \sum_{i=1}^{N} t_{u_i}^2 + \sum_{j=1}^{M} t'_{j=1}^2$$
 (6)

■ Taking derivatives with respect to t_{u_i} and setting to zero gives:

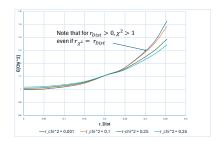
$$\frac{\partial(-2LnL)}{\partial t_{u_i}} = 0 \implies t_{u_i} = \frac{\sigma_{u_i}(y_i - d_i - \sum_j \beta_{ij}t_j')}{\sigma_i^2 + \sigma_{u_i}^2}$$
(7)

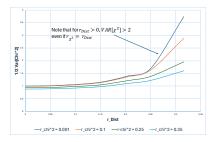
Substituting equation (7) into (6) gives our expected Gaussian formulation:

$$-2LnL = \sum_{i=1}^{N} \frac{(y_i - d_i - \sum_j \beta_{ij} t_j')^2}{\sigma_i^2 + \sigma_{u_i}^2} + \sum_{i=1}^{M} t'^2$$
 (8)

Expectation and Variance of χ^2 as a Function of r

Let's consider the case: $y_i = d_i + \sigma_i z_i + \sigma_{u_i} t_{u_i}$, with $z_i \sim N(0, 1)$, $t_{u_i} \sim t(0, \nu = 1/2r_{Dist}^2)$. i.e. focus on the uncorrelated systematic behaviour $(\beta_{ij} = 0)$.





Graph of $E[\chi^2]$ as a Function of r_{Dist} for 4 different r_{χ^2} ($\sigma_i = \sigma_{u_i} = 1$)

Graph of $Var[\chi^2]$ as a Function of r_{Dist} for 4 different r_{χ^2} ($\sigma_i = \sigma_{u_i} = 1$)

Standard Deviation of the Simple Mean as a Function of *r*

- Consider the case: $y_i = d_i + \sigma_i z_i + \sigma_{u_i} t_{u_i}$, with $z_i \sim N(0, 1)$, $t_{u_i} \sim t(0, v = 1/2r_{Dist}^2)$. Also let $E[d_i] = d$
- The standard deviation of the simple mean, $y_{mean} = \sum_{i=1}^{N} y_i/N$, is:

$$\sigma_{\textit{Mean}} \approx \frac{\sqrt{\sum_{i=1}^{\textit{N}} \sigma_i^2 + \sigma_{\textit{U}_i}^2 \nu/(\nu-2)}}{\textit{N}} = \frac{\sqrt{\sum_{i=1}^{\textit{N}} \textit{E}[\chi_i^2(\textit{r}_{\chi^2} \rightarrow 0)](\sigma_i^2 + \sigma_{\textit{U}_i}^2)}}{\textit{N}}$$

■ Table showing σ_{mean} as a function of r and N (with $\sigma_i = \sigma_{u_i} = 1$)

	r _{Dist}	N=2	N=3	N=5	N=10	N=100	N=500	$\frac{\sigma_{r_{Dist}}}{\sigma_{(r_{Dist}=0.001)}} N = 500$
ſ	0.001	0.995	0.819	0.630	0.449	0.142	0.064	1.000
ı	0.100	0.991	0.814	0.641	0.452	0.143	0.064	1.005
	0.250	1.092	0.884	0.679	0.481	0.152	0.069	1.077
ı	0.300	1.122	0.926	0.705	0.504	0.161	0.071	1.108
	0.408	1.417	1.148	0.901	0.637	0.197	0.089	1.393

■ This table gives the standard deviation for the fitted mean if $r_{x^2} = 0.0001$

Standard Deviation of the Fitted Mean as a Function of r

- What happens if we minimize the χ^2 , calculated with $r_{\chi^2} = r_{Dist}$, with respect to our mean?
- Table showing σ_{FIT} as a function of r and N (with $\sigma_i = \sigma_{u_i} = 1$)

r	N=2	N=3	N=5	N=10	N=100	N=500	$\frac{\sigma_{FIT}}{\sigma_{r_{Dis}=r_{v^2}=0.001}}$ N=500
0.001	0.995	0.819	0.630	0.449	0.142	0.064	1.000
0.100	0.991	0.814	0.641	0.452	0.143	0.064	1.004
0.250	1.092	0.883	0.675	0.479	0.150	0.068	1.069
0.300	1.122	0.916	0.697	0.493	0.157	0.069	1.087
0.408	1.417	1.162	0.809	0.547	0.169	0.076	1.186

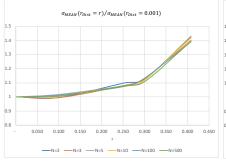
Data obtained using MC

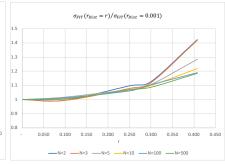
■ For Gaussian statistical errors and t-distributed uncorrelated systematic errors:

$$\sigma_{FIT} = \sqrt{\sum_{i=1}^{N} E\left[\chi_i^2(r_{\chi^2} = r_{Dist})\right](\sigma_i^2 + \sigma_{u_i}^2)} / N$$

Standard Deviation of the Mean Fitted Mean

- Graph on left shows ratio of $\frac{\sigma_{Mean}}{\sigma_{Mean}(r_{Dist}=0.001)}$ as a function of r and N.
- Graph on right shows ratio of $\frac{\sigma_{Fit}(r_{Dist}=r_{\chi^2}=r)}{\sigma_{Fit}(r_{Dist}=r_{\chi^2}=0.001)}$ as a function of r and N.





Expectation and Variance of χ^2 as a Function of r

■ Consider the case of N observables each with a Gaussian statistical and M t-distributed correlated systematic errors :

$$y_i = d_i + \sigma_i z_i + \sum_{j=1}^{M} \beta_{ij} t'_j$$
 $z_i \sim N(0, 1), t'_j \sim t(0, \nu = 1/2r_{Dist}^2)$

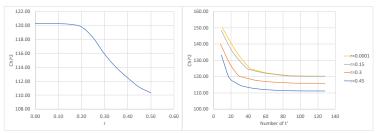
■ In the case where $r_{Dist} = r_{\chi^2}$, and $\sigma_i = \beta_{ij} = 1$:

						$\sigma_{\varphi_{MEAN}} =$			$\sigma_{\varphi_{FIT}}$
N	М	r	ν	$E[\chi^2(d_i)]$	σ_{χ^2}	$\sigma_{FIT(r_{\chi^2}=0.001)}$	$\sigma_{\varphi_{FIT}}$	$\sigma_{\varphi_{FIT}}/\sigma_{\varphi_{MEAN}}$	$\sigma_{\varphi_{FIT}(r_{Dst}=r_{\chi^2}=0.001)}$
2	2	0.001	500000	1.99949	2.05734	1.58114	1.58114	1.000	1.000
2	2	0.25	8	2.28779	2.31064	1.78103	1.78970	1.005	1.132
2	2	0.40824829	3	2.87634	2.98990	2.51644	2.32738	0.925	1.472
5	5	0.001	500000	4.99873	3.20452	2.28036	2.28036	1.000	1.000
5	5	0.25	8	5.42717	3.44951	2.62217	2.62208	1.000	1.150
5	5	0.40824829	3	6.53625	4.49232	3.81179	3.51314	0.922	1.541
10	5	0.001	500000	9.99746	4.58094	2.25832	2.25833	1.000	1.000
10	5	0.25	8	10.47021	4.68864	2.64291	2.63296	0.996	1.166
10	5	0.40824829	3	11.61824	5.53776	4.08220	3.48161	0.853	1.542
10	10	0.001	500000	9.99746	4.53088	3.17806	3.17806	1.000	1.000
10	10	0.25	8	10.37782	4.69332	3.67337	3.64109	0.991	1.146
10	10	0.40824829	3	11.91221	5.81006	5.40928	4.72917	0.874	1.488

where $E[\chi^2(d_i)]$ means that $E[\chi^2]$ calculated with a mean equal to d_i

ATLAS W,Z Data analysis3

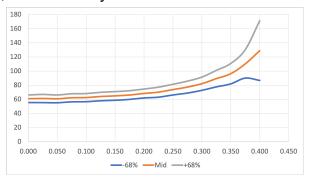
This very precise data gives strong constraint on the strange quark. However fit is poor $\chi^2/N_{pt}\sim$ 1.9 for MSHT20 (NNLO). $N_{pt}=61$



- Graph on the left shows the χ^2 as a function of relative error,r.
- Graph on the right shows how χ^2 is impacted by only considering the N largest t' for different relative errors: r = 0.0001, r = 0.15, r = 0.3, r = 0.45

³ https://www.hepdata.net/record/ins1502620 Tables 9 - 15

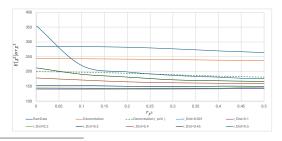
ATLAS W,Z Data analysis



- Graph shows the χ^2 calculated using r = 0.001 as a function of relative error, r_{Dist} of the simulated underlying systematic errors.
- Included is both the Expectation and the standard deviation
- For a χ^2 of 120 $r \approx 0.4$

ATLAS 7 TeV Inclusive Jet Distributions Analysis

- This ATLAS data⁴, combined with availability of NNLO corrections provides constraints on the Gluon PDF at high x.
- Graph shows the χ^2 or $E[\chi^2]$ as a function of relative error, r_{χ^2} .
 - Raw data refers to just the raw data provided by ATLAS. 140 Data points.
 - Difficult to fit all rapidity bins simultaneously. De-correlation refers to χ^2 calculated with small number (3) of the "two point" systematic uncertainties de-correlated ⁵
 - Other lines show the $E[\chi^2]$ using pseudo data produced using $r_{Dist} = 0.0001, 0.1, 0.2, 0.3, 0.4, 0.45, 0.5$.

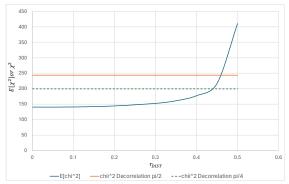


⁴https://www.hepdata.net/record/ins1325553 - tables 7-12 for "R=0.6"

⁵MSHT20 arXiv:2012.04684

ATLAS 7 TeV Inclusive Jet Distributions Analysis

- Graph shows $E[\chi^2]$, calculated with $r_{\chi^2} = 0.00001$, where systematic errors are sampled from t-distribution with d.o.f $1/2r_{Dist}^2$.
- Line at 243.43 is χ^2 calculated using $r_{\chi^2} = 0.0001$ for de-correlated data.



De-correlation

- Sometimes we use decorrelation techniques for systematic errors.
- E.g. would be when a systematic error is the calculated as the difference between two different Monte Carlo runs with different input parameters.
- For the ATLAS 7 TeV Jet Data, as is done in the MSHT20 paper, we could use a paramaterisation which allow data points that are distant in (y_j, p_{\perp}^j) space to have different systematic variations:

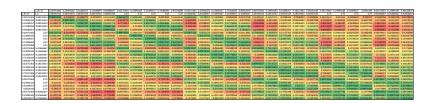
$$\begin{aligned} x_{p_{\perp}} &= \frac{\log(p_{\perp}^{j}) - \log(p_{\perp,min}^{j})}{\log(p_{\perp,max}^{j}) - \log(p_{\perp,min}^{j})} \\ x_{y} &= \frac{y_{j} - y_{j,min}}{y_{j,min} - y_{j,max}} \\ r &= \frac{1}{\sqrt{2}} \sqrt{x_{\perp}^{2} + x_{y}^{2}}, \, \varphi = \arctan\left(\frac{x_{y}}{x_{p_{\perp}}}\right) \\ \mathcal{L}_{trig}(z, z_{min}, z_{max}) &= \cos\left[\pi\left(\frac{z - z_{min}}{z_{max} - z_{min}}\right)\right] \end{aligned}$$

$$\begin{split} \beta_{i}^{(1)} &= L_{trig}(r, 0, 1).L_{trig}\left(\varphi, 0, \frac{\pi}{2}\right)\beta_{i}^{tot} \\ \beta_{i}^{(2)} &= \sqrt{1 - L_{trig}(r, 0, 1)^{2}}.L_{trig}\left(\varphi, 0, \frac{\pi}{2}\right)\beta_{i}^{tot} \\ \beta_{i}^{(3)} &= L_{trig}(r, 0, 1).\sqrt{1 - L_{trig}\left(\varphi, 0, \frac{\pi}{2}\right)^{2}}\beta_{i}^{tot} \\ \beta_{i}^{(4)} &= \sqrt{1 - L_{trig}(r, 0, 1)^{2}}.\sqrt{L_{trig}\left(\varphi, 0, \frac{\pi}{2}\right)^{2}}\beta_{i}^{tot} \end{split}$$

■ If we implement this for the , then if r = 0.0001, then the $\chi^2 = 243.43$.

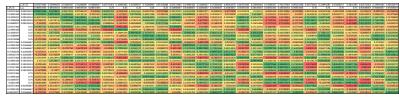
Correlation Structure

- We can determine this by looking at the resulting correlation structure obtained from Monte Carlo.
- For the MSHT20 decorrelation we have the simplified correlation matrix:



Correlation Structure

- So what happens if we change the $\pi/2$ to $\pi/4$?
- Firstly there is a big fall in χ^2 . It goes from 243.43 to 199.18
- The Correlation matrix becomes:



■ In some parts of the matrix this looks better, but in others worse than the desired outcome!

Conclusions

- We have shown how we can incorporate Errors on Errors into the calculation of a χ^2
- Expected χ^2 and Variance of χ^2 increase as the relative errors of the systematic errors increase
- We have noted that for both data sets $r \approx 0.4$. If we compare the expected standard deviation of the mean, calculated with $r_{\chi^2} = 0.001$, where the systematic errors have an $r_{Dist} = 0.4$ to that where $r_{Dist} = 0.001$ we obtain a ratio of approx. 1.2 1.5. This is suggestive of using a tolerance in the region of 1.2 1.5 in these test cases.
- When de-correlating systematic errors we need to be incredibly careful about the correlation matrix that we are producing



Back Up Slides

Closer Look at the Correlation Matrix - $\pi/2$ versus $\pi/4$ In some parts of the correlation matrix using $\pi/2$ looks better, but in other parts it looks worse.



 $\pi/2$

Better												
	x_{P_T} \	0.02572464	0.23994183	0.51009257	0.74286895	0.95880057	0.02572464	0.23994183	0.51009257	0.74286895	0.93724088	
x_{P_T}	x_y	0.08333333	0.08333333	0.08333333	0.08333333	0.08333333	0.25	0.25	0.25	0.25	0.25	
0.02572464	0.08333333	0.99974556	0.9228621	0.49272974	0.07584232	-0.240455	0.65907332	-0.2405758	0.39051862	0.02322744	-0.3757966	
0.23994183	0.08333333	0.9228621	0.99974549	0.64364632	0.28738736	-0.0015913	0.60011925	-0.1478024	0.6775356	0.38337488	-0.0189196	
0.51009257	0.08333333	0.49272974	0.64364632	0.99974564	0.85380853	0.52406367	0.80746022	-0.6923689	0.38290406	0.65961034	0.4934031	
0.74286895	0.08333333	0.07584232	0.28738736	0.85380853	0.99974562	0.88354433	0.45112934	-0.5427014	0.17837245	0.65642429	0.72844584	
0.95880057	0.08333333	-0.240455	-0.0015913	0.52406367	0.88354433	0.99974552	-0.0088366	-0.1829543	0.06056808	0.535064	0.76717266	
0.02572464	0.25	0.65907332	0.60011925	0.80746022	0.45112934	-0.0088366	0.99974556	-0.8614181	0.12004887	0.23849793	-0.0207453	
0.23994183	0.25	-0.2405758	-0.1478024	-0.6923689	-0.5427014	-0.1829543	-0.8614181	0.99974559	0.28894148	-0.1066135	-0.0796406	
0.51009257	0.25	0.39051862	0.6775356	0.38290406	0.17837245	0.06056808	0.12004887	0.28894148	0.99974547	0.76794774	0.44568291	
0.74286895	0.25	0.02322744	0.38337488	0.65961034	0.65642429	0.535064	0.23849793	-0.1066135	0.76794774	0.99974561	0.88563822	
0.93724088	0.25	-0.3757966	-0.0189196	0.4934031	0.72844584	0.76717266	-0.0207453	-0.0796406	0.44568291	0.88563822	0.99974545	

 $\pi/4$

Treating our r_i , r_{u_i} and r' as 0 Correlated - Model 2

■ In this scenario we obtain the Loglikehihood equation:

$$-2LnL = \sum_{i=1}^{N} \left(\frac{y_i - t_i - \sigma_{u_i} r_{u_i} - \sum_{j} \beta_{ij} r_j'}{\sigma_i} \right)^2 + \sum_{i=1}^{N} (\nu + 1) Ln \left(1 + \frac{r_{u_i}^2}{\nu} \right) + (\nu + M) Ln \left(1 + \frac{\sum_{j}^{M} r_j'^2}{\nu} \right)$$
(9)

- Again we obtain cubic equations for r_{u_i} and r'_i .
- The equation for r_{u_i} can be solved analytically whilst solving for r'_j numerically.
- Model 1 and Model 2 have a different dependence on ν . In order to make Model 1 and Model 2 closer we shall let $\nu \to M\nu$.

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