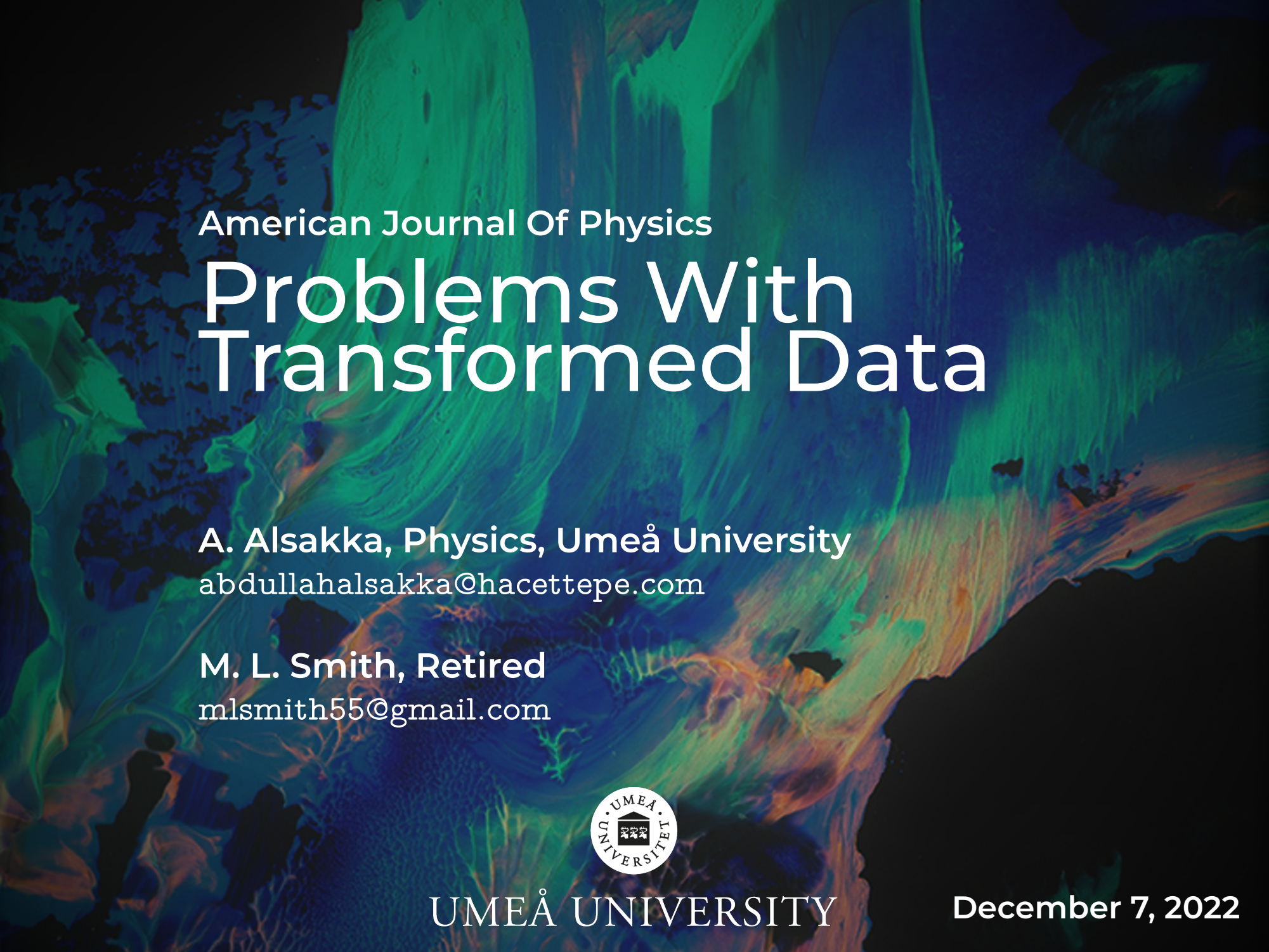

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Problems With Transformed Data

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Contents

Introduction

Scientists commonly use graphs to represent observations and mathematics to explain correlations. The experiment of Galileo is a good example where free fall distance is correlated to time and presents a beautiful graph. It is now common to model mathematical descriptions then choose the best model using statistics as a guide.

It is important to select the proper metric for data analysis. One would select meters and seconds for the Galileo experiment; miles and days would be inappropriate.

We explore some problems when inappropriate metrics are chosen. One example follows cancer cell replication over time, our second example presents astronomical observations of distant supernovae. We find that investigators select the proper metrics for one experiment but inappropriate metrics for the second.

Introduction

A common fault is choosing data without a metric or transforming data by applying the log function, log(x), then using the "new" data. Some reasons why using log(data) often leads to incorrect results:

1. Data are measured using metrics (m, km, seconds, etc.), however $\log(x)$ has no metric.
2. Standard deviations, log(σ), are distorted often becoming worse the further the measurement is taken from the origin.
3. The best data pair, sometimes the origin (at 0,0) without significant error, cannot be used because $\log(0) = -\infty$. Exclusion of any data pair with insignificant error can never be justified.
4. Since the σ values are distorted, computerized goodness of fit estimates are improperly estimated; χ^2 and r^2 are often incorrect, complicating model discrimination.

Standard Deviations

The σ, the standard deviation, is an estimate of the uncertainty of the dependent measurement. This usually means the correct value has a $\approx 67\%$ probability of residing between the upper and lower limits of σ, presuming a Gaussian distribution of "real" values.

Consider a function of $f(x)$ where the x value has an estimated error of $\pm x_{\text{err}}$. Our error for the y values at any arbitrary x value is

$$y_{\text{err}} = \frac{f(x + x_{\text{err}}) - f(x - x_{\text{err}})}{2}$$

Therefore the standard deviation, σ, is an estimate of how much the y value might deviate from the mean, so $\sigma = y_{\text{err}}$. The dependent variable is usually chosen as the variable with greater σ and the $\sigma_{(x)}$ is often considered to be negligible to ease calculations.

Chi-squared test, χ^2

Pearson's χ^2 is a commonly used measure of a model compliance with the data and calculated as

$$\chi^2 = \sum \left(\frac{(\text{Observed value} - \text{Expected value})^2}{\text{Expected value}} \right).$$

A smaller χ^2 usually indicates a better model.

Some investigators use the *reduced* χ^2, which is simply the "normalized" χ^2 as

$$\chi^2_{red} = \chi^2 / (N - P)$$

where N are the number of data pairs and P the parameter count. Models sporting many parameters will display larger values of χ^2 and χ^2_{red}.

r-squared test, r^2

The r-squared, r^2, statistic is a commonly used measure of the correlation between the dependent and independent variables. It is calculated as

$$r^2 = 1 - \frac{\sum(y_{\text{observed}} - y_{\text{expected}})^2}{\sum(y_{\text{observed}} - y_{\text{mean}})^2}.$$

Formally r^2 only applies to linear models, for more general application the *adjusted* r^2 is used as

$$r^2_{adj} = 1 - \frac{(1 - r^2)(N - 1)}{(N - P - 1)}$$

where N are the number of data pairs and P is the parameter count. There are many other statistical tests which are useful to estimate model worth, the F-test being very good.

Programs

The popular Python 3 programming language used here, is available for free and one helpful website is

https://www.anaconda.com/products/distribution

We checked our routines with the Jupyter Notebook and Spyder IDE using both Apple® Macintosh and Windows® 11 on a PC laptop. We have saved the publicly available data as .csv files for use with *scipy*, *pandas* and *numpy* Python libraries.

Where to find the data? Where to find the programs?

All programs and data are available in a GitHub repository -

https://github.com/MLSResearchGroup/About-Transforming-Data

Data

Both sets of native and transformed data are from online sources and articles [1], [2].

The first experiment are counts of cancer cells every 4 hours for 236 hours during replication [1]. Ten independent counts were made at each time and the mean and σ were calculated using a spreadsheet and saved in the .csv file.

For the second set, we use observational data of supernovae type Ia (SNe Ia) emissions reported by the Riess team of astronomers [2]. We use the values of *mag* (*distance mag*) and σ as given and "back-calculate" the supernovae distances, D_L, and related σ values using a spreadsheet and saved in the GitHub repository.

Cancer cell replication is a good example of exponential growth. We model the cell count increase over time as

Exponential model (Exp)

$$N(t) = N_0 e^{\beta t} \tag{1}$$

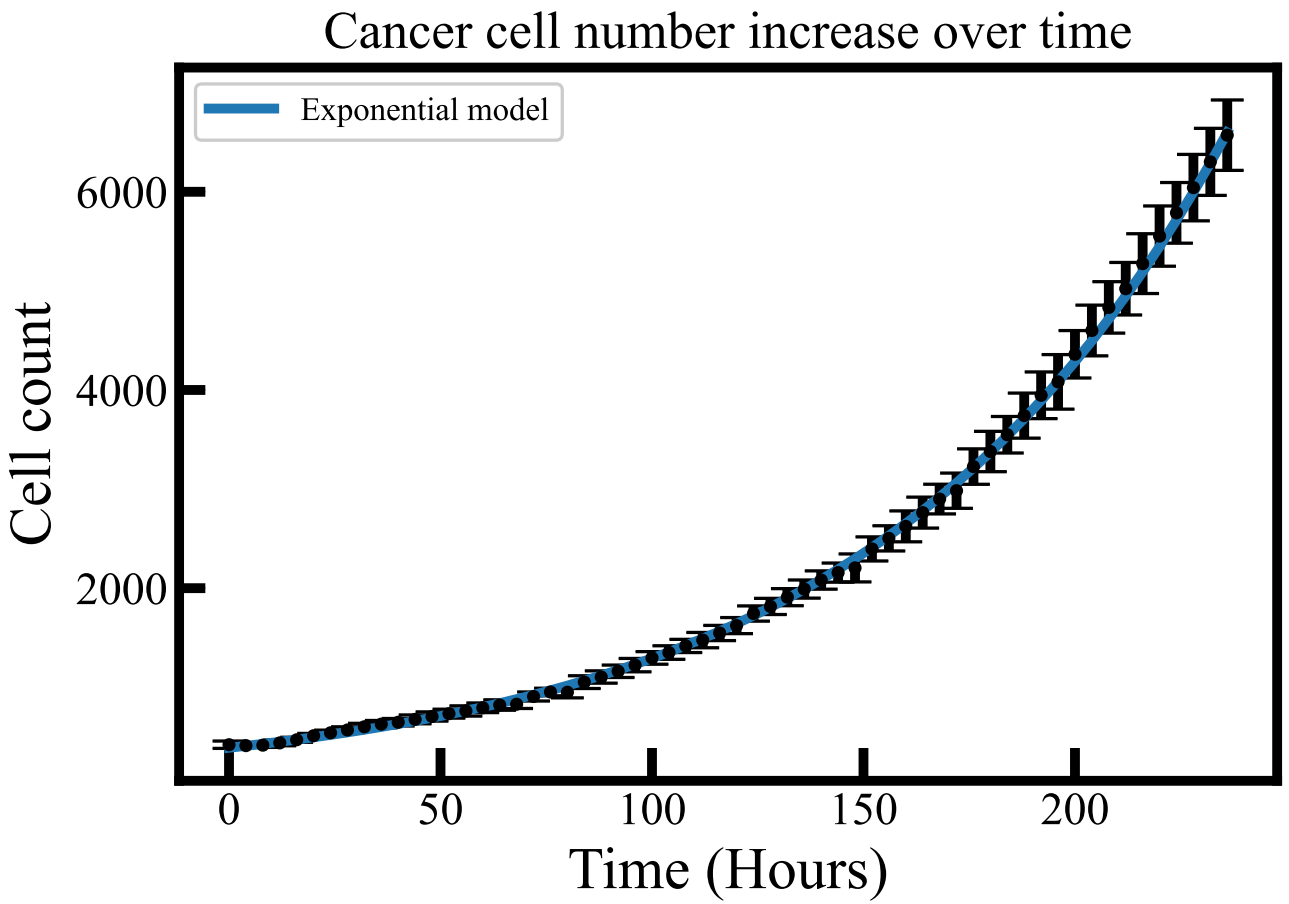
Here N_0 is the initial cell number, β the replication rate and t, the time (hours). To transform the dependent data we take the natural logarithm of equation (1) on both sides yielding

logarithmic model (Log)

$$\ln[N(t)] = \ln N_0 + \beta t \tag{2}$$

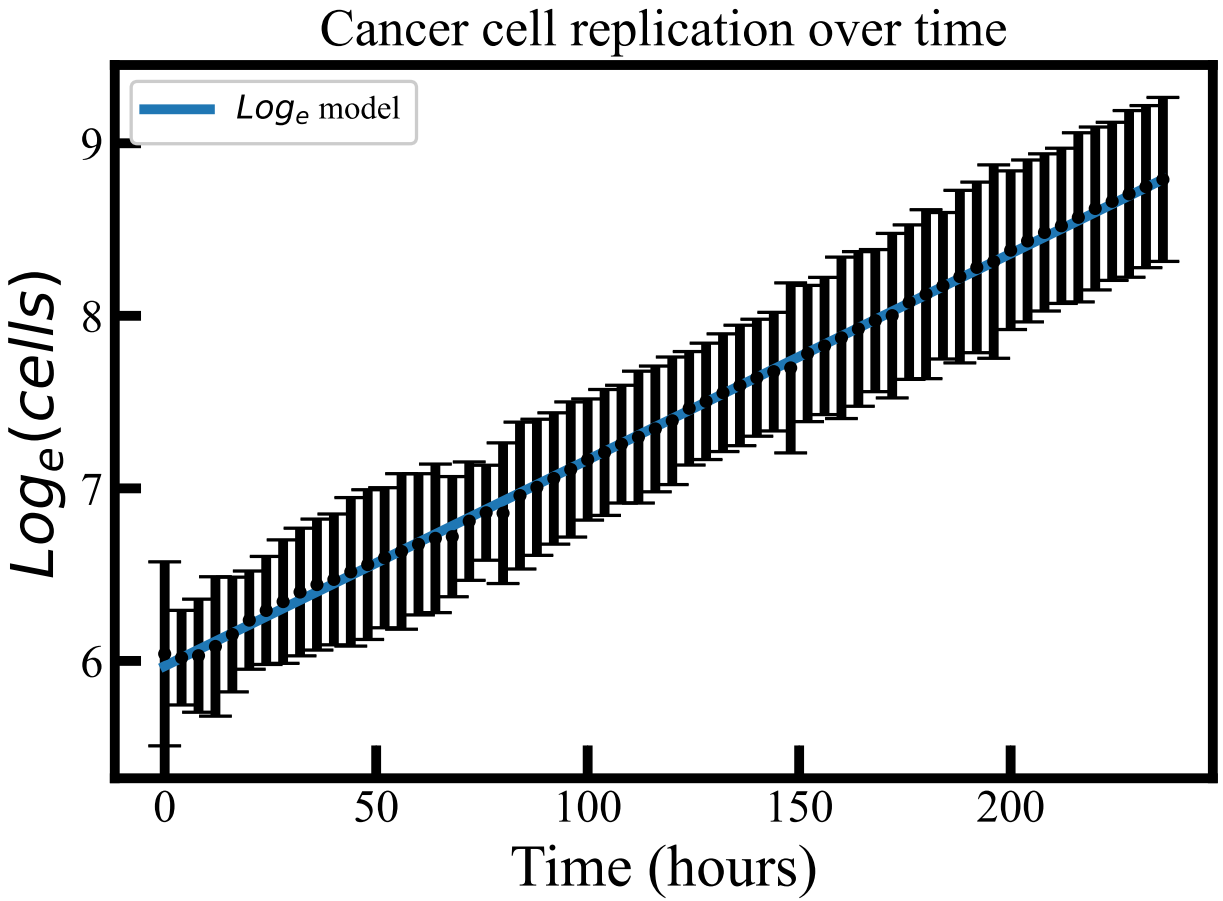
our logarithmic model is an example of coordinate transformation; the y-axis data are transformed into log_e*(data)*.

Cancer Cell Replication
Exponential Model Plot



Note the steady increase of standard deviation with time.

Cancer Cell Replication
Log Model Plot



The semi-log plot example. Note the smaller increase of $Log_e(\sigma)$ with time.

Cancer Cell Replication
Results

Table: Results from the Exp and Log models of cancer cell replication data using curve_fit regression routine. Both calculations use relative weights of σ values.

Model	N_0 (initial cell count)	β (hour^{-1}) growth rate	r^2_{adj}	χ^2
Exp	389.6$\pm$2.3	0.012$\pm 4E^{-5}$	0.9995	40.6
Log_e	391.4$\pm$1.0	0.012$\pm 5E^{-5}$	0.9992	0.005

- Both r^2_{adj} values are $\approx$1 but χ^2 values are dissimilar; these two regressions should be comparable but are not [3-6]
- Distortion of the $Log_e(\sigma)$ values is reflected in the very small χ^2; warning that these results are suspect
- The value for N_0 are smaller than the cell count at $t = 0$, indicating some cells died during experiment initiation

Astrophysicists commonly correlate galactic distances with redshifts (*z*). Strong correlation is considered evidence supporting claims about Universe expansion rate, spacetime geometry, matter density, dark matter and dark energy.

Intergalactic distances are often measured from light intensity, use a scale termed *mag* or *distance mag*. This historic method follows the logarithmic scaling of luminosity as perceived by the human eye.

The actual luminosity distance is based better on D_L, as parsec (pc), kiloparsec (Kpc) or megaparsec (Mpc) which are measures of large distances. The best data currently comes from measuring the luminosity of distant supernovae (SNe Ia) explosions and the associated galaxy redshift, z. These emissions are considered standard candles.

Supernovae Type Ia Cosmology

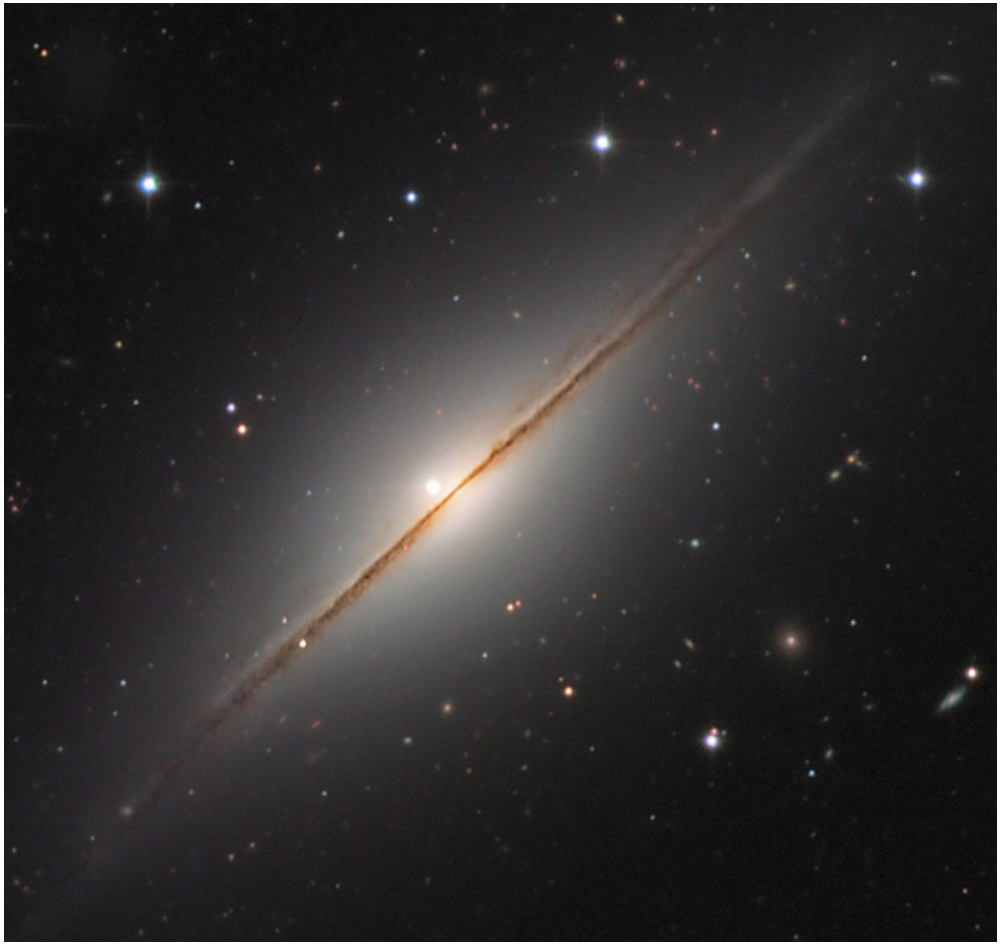


Figure: The supernova near the Little Sombrero galaxy. The bright light just to the left of the galactic center is a type Ia supernova as recorded July 17, 2021. Image from NASA.

For the SNe Ia data the mag is a function of D_L as

$$mag = 5 \log_{10} D_L + 25$$

and the luminosity distance, D_L in Mpc units, is "back-calculated" from *mag* often as

$$D_L = 10^{(mag-25)/5}.$$

Astrophysicists use the redshift, z, as a measure of galactic recession velocity, this is easy to measure with little error. We calculate the relative recession velocity using

$$\xi = \frac{1}{1+z} = \frac{\nu}{\nu_0}$$

where ξ is the ratio of the observed, lower frequency, ν, over ν_0 - the frequency unmodified by the Doppler effect. The value ξ is often termed the expansion factor or sometimes a.

The Einstein-DeSitter (E-DS) model considers our Universe being primarily matter without spacetime or dark energy [7]. To find the local Hubble constant, H_0, with mag and z data we use

magE-DS model

$$mag = 5\log_{10}\left[\frac{c(1+z)}{H_0}\sinh\left(\frac{z}{1+z}\right)\right] + 25.$$

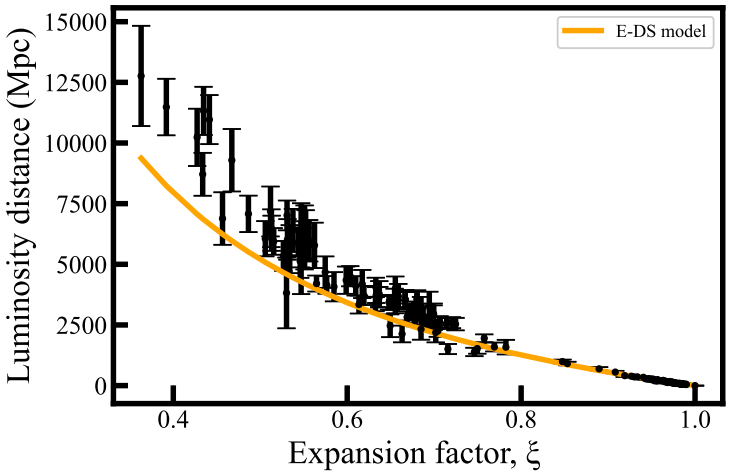
With the D_L and ξ data we use the simpler

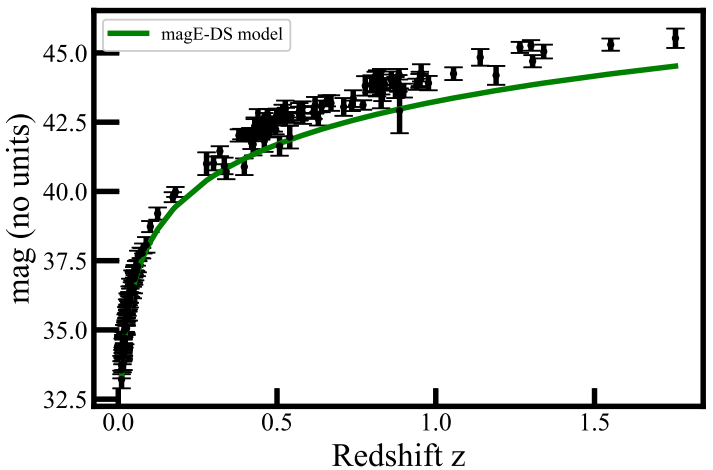
E-DS model

$$D_L = \frac{c}{H_0\xi}\sinh\left(1-\xi\right)$$

here c is lightspeed as km s^{-1} and H_0 as km s^{-1} Mpc^{-1}.

Supernovae Type Ia Cosmology
E-DS model, using "gold" data from Riess et al. 2004





The E-DS model was suggested before the tremendous size of our Universe was known. The best data available to Einstein was published by Hubble in 1929 [8].

Physicists now use *normalized* parameters to calculate properties of our Universe: for matter density we use Ω_m; Ω_k describes the portion which is not matter but spacetime; Ω_Λ to describe galactic motions and Universe expansion [9].

normalized Ω parameters

Normalized parameters means the parameters sum to 1; keep these relationships in mind

$$\Omega_m + \Omega_\Lambda = 1$$

for the ΛCDM model, the *standard model* of cosmology and

$$\Omega_m + \Omega_k = 1$$

for the *arctanh* models (**see appendix**) ; the Universe without dark energy. Remember that $1 - \Omega_m = \Omega_\Lambda$ or $1 - \Omega_m = \Omega_k$.

We write the luminosity distance, D_L, in term of the normalized parameters and ξ for the *standard model* as

ΛCDM model, distance vs. recession velocity

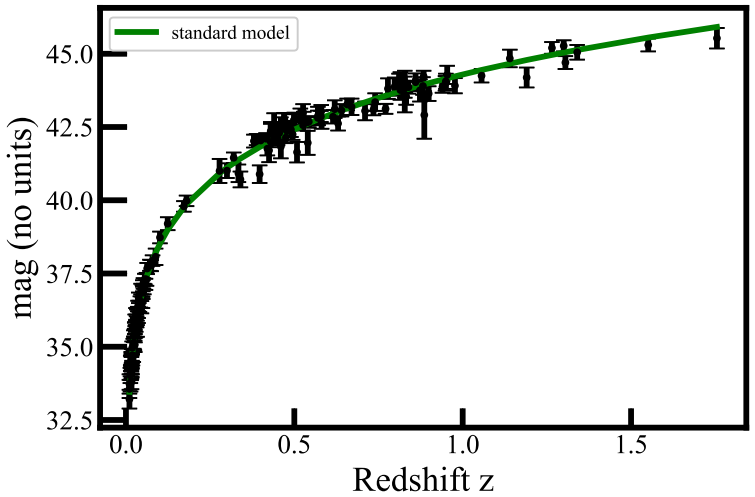
$$D_L = \frac{c}{H_0 \xi} \sinh \left\{ \int_{\xi_1}^{1} \frac{d\xi}{\xi \sqrt{\frac{\Omega_m}{\xi} + \Omega_\Lambda \xi^2}} \right\}$$

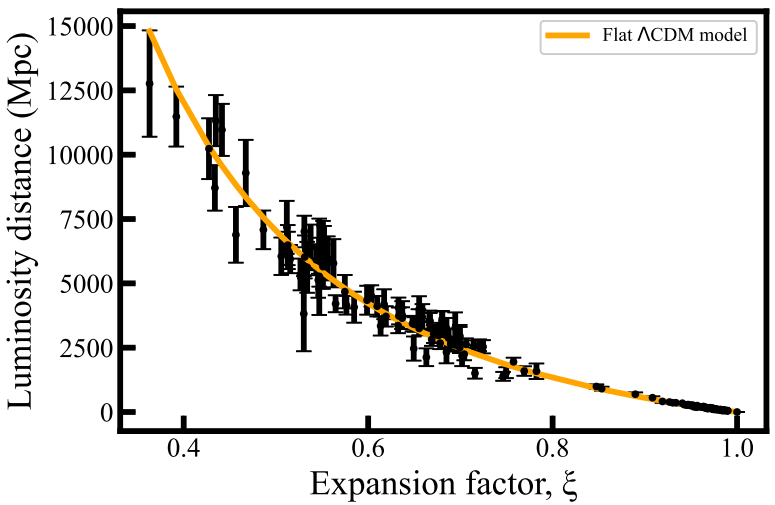
This integral cannot be calculated analytically, so we must use numerical integration methods in Python. We also write the *standard model* in terms of *mag* and redshift z as

The standard model of cosmology, mag vs. redshift [2]

$$mag = \frac{c(1+z)}{H_0} \sinh \left\{ \int_{0}^{z} \frac{dz}{\sqrt{(1+z)^2(1+\Omega_m z) - z(2+z)(\Omega_\Lambda)}} \right\}$$

Supernovae Type Ia Cosmology
The *standard* and ΛCDM models





Note the difference between the size of σ values with plots.

Table: Results from the Einstein-DeSitter, *standard* and *arctanh* models using the gold SNe Ia data with curve_fit regression routine. All calculations use relative weights of σ values.

model	H_o (km s^{-1} Mpc^{-1})	Ω_m with Ω_k or (Ω_Λ)	r^2_{adj}	χ^2_{red}
E-DS	57.4$\pm$0.8	-	0.887	166.6
*mag*E-DS	54.8$\pm$0.8	-	0.988	0.0043
ΛCDM	64.8$\pm$0.9	(0.48$\pm$0.05)	0.968	45.1
standard	63.8$\pm$0.8	(0.47$\pm$0.05)	0.995	0.0019
model				
arctanh	63.9$\pm$0.8	0.008$\pm$0.075	0.965	47.5
*mag*arctanh	62.7$\pm$0.8	0.001$\pm$0.075	0.994	0.0020

The H_o of the E-DS models are significantly smaller than the *standard* and *arctanh* models (**appendix**). Note that r^2_{adj} and χ^2_{red} differ between the *mag* vs. *z* and D_L vs. ξ calculations.

- The E-DS model functions well for nearby distances but fails at larger distances
- The Hubble constant from the E-DS calculations is ≈55-58 km s^{-1} Mpc^{-1}, much lower than recent estimates of ≈62-74 [10]
- The values for Ω_m from the *standard* and ΛCDM models are significantly higher than the *arctanh* models
- The Ω_k is calculated to be very large (≈1) for the *arctanh* model but presumed to be ≈0 for the *standard* model
- Because σ values are smaller after log transformation, the values of r^2_{adj} and χ^2_{red} should be considered doctored
- Parameter values and statistics should not differ between metrics but the statistics are badly distorted by the log(data) transformation

Conclusions

We demonstrate that data transformation shall be avoided

- The example using cancer cell counts during replication showed that transforming good data, especially the σ values, can lead to faulty statistics and is a waste of time
- Transforming data just to visualize a straight line may lead to incorrect results
- The σ values associated with SNe Ia *mag* values [2,11] suffer artificial contraction
- Discarding the origin when employing the log(data) transformation cannot be justified (**appendix**)
- Calculated parameters and standard deviations should be similar using either metric values or transformed values but are not

*The statistics calculated using these data do not necessarily support a preference for the *standard* model over the *arctanh* model but only over the E-DS model

Questions

Some questions may be asked

- Derive the well known equation for standard deviation

$$\sigma = \sqrt{\frac{\sum(x_i - \mu)}{N}}$$

  where μ is the mean, x_i the observed values and N the number of observations, from the equation on page 5.
- Why does the Log model presents a slightly better estimate of initial cell count (420) than the Exp model?
- Does this justify using a Log model, or is it just happenstance?
- Evaluate the local Hubble law $\frac{c}{\xi} = H_0 D_L$ beginning with the E-DS or arctanh model?
- Which universe model do you think is closer to reality? Why?

Questions

Some more questions

- The expansion factor, $\xi = 1$, is our relative recession velocity and the position of our earth, $D_L = 0$, a certainty. Now consider our situation when the recession velocity $z \to 0$ and *mag*$= -\infty$.
  - Is it justified to discard the position of the earth, the only point with full certainty, when using the *mag* models?
  - Is the redshift, *z*, a useful transform of ξ? (**appendix**)
- The σ values associated with the *mag* data are relatively smaller than the σ values associated with D_L. Do we always want smaller errors, explain?
- When Einstein derived his cosmological model (E-DS), it was thought the universe was only the Milky Way and all stars are motionless.
  - Do you think this is reflected in the E-DS model?
  - Historical question - Why did Einstein and Stephen Hawking consider our Universe matter dominated?
- Difficult question - edit either the arctanh or magarctanh model to evaluate the data with one more free parameter - the Ω_k. The code will now have 3 parameters. If successful note the standard deviations.

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The *arctanh* model describes a universe containing matter with non-Euclidean spacetime but without the cosmological constant (no dark energy). The relationship takes the form

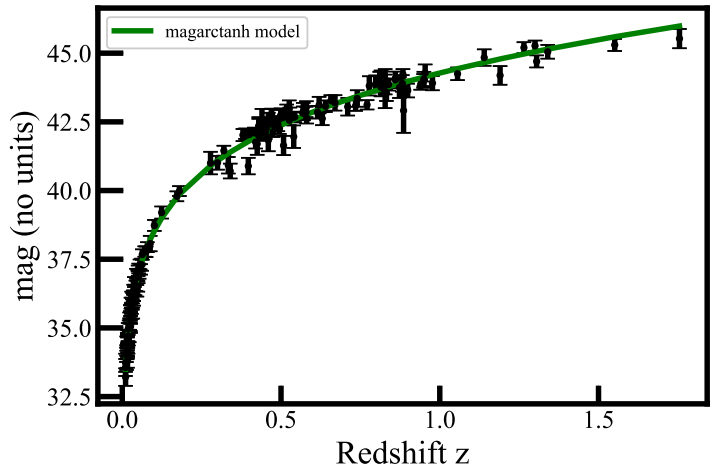
arctanh model, distance vs. recession velocity

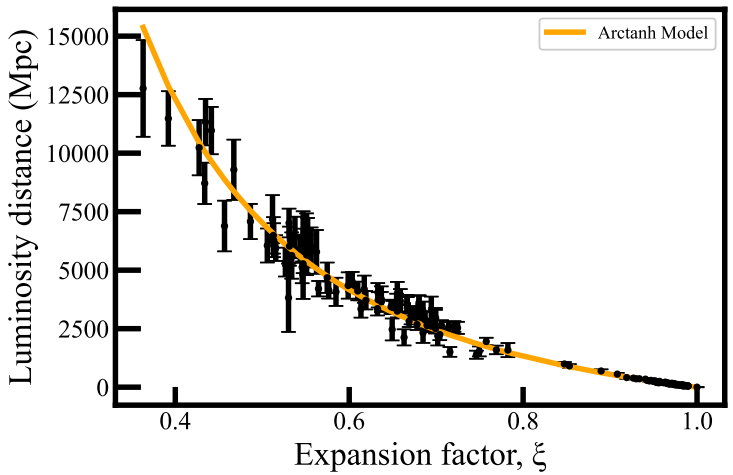
$$D_L = \frac{c}{H_0 \xi \sqrt{|\Omega_k|}} \sinh\left\{ \sqrt{|\Omega_k|} \int_{\xi_1}^{1} \frac{d\xi}{\xi \sqrt{\frac{\Omega_m}{\xi} + \Omega_k}} \right\}$$

and this can be integrated to become

$$D_L = \frac{c}{H_0 \xi \sqrt{|\Omega_k|}} \sinh\left\{ 2\left(\operatorname{arctanh}(\sqrt{|\Omega_k|}) - \operatorname{arctanh}\left(\frac{\sqrt{|\Omega_k|}}{\sqrt{\frac{\Omega_m}{\xi} + \Omega_k}} \right) \right) \right\}$$

Supernovae Type Ia, appendix
Arctanh model, *mag vs z* and D_L vs ξ plots





These figures are similar in appearance to the *standard* and ΛCDM model figures though the models are quite different.

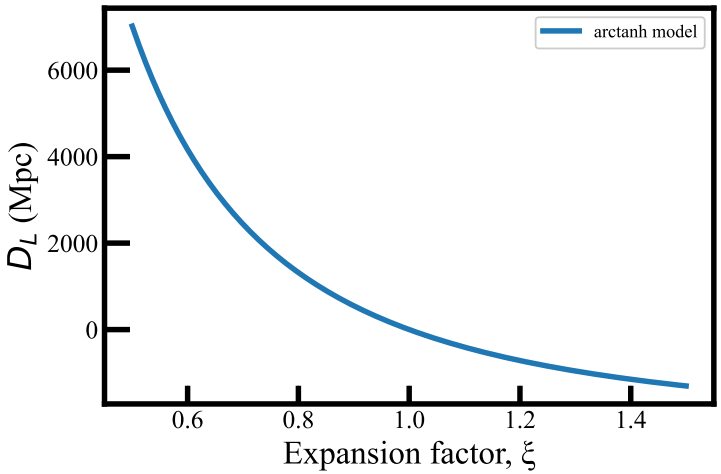
Predicting our present & future
The *arctanh* model success and *magarctanh* failure

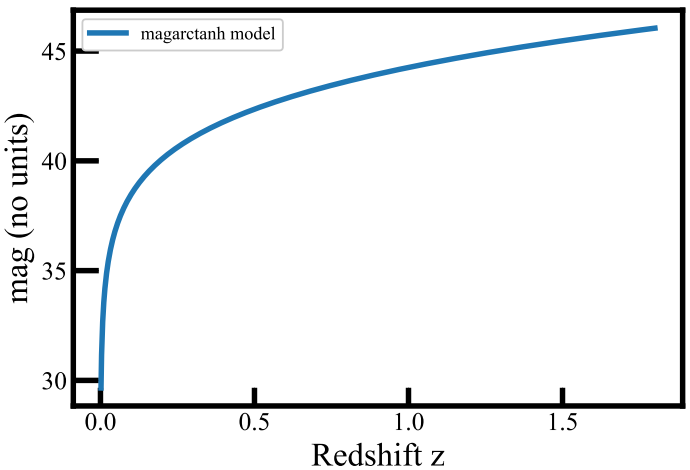
A strength of science is the ability to predict the future and describe the present. Calculation of the origin at $z = 0$ is impossible for the *mag*arctanh model

- the log of our position at the origin 0 is $-\infty$
- but our position is known with 100% certainty

Our present and future conditions are presented in the next two figures. The failure of the *mag*arctanh model is also observed for the *standard* model.

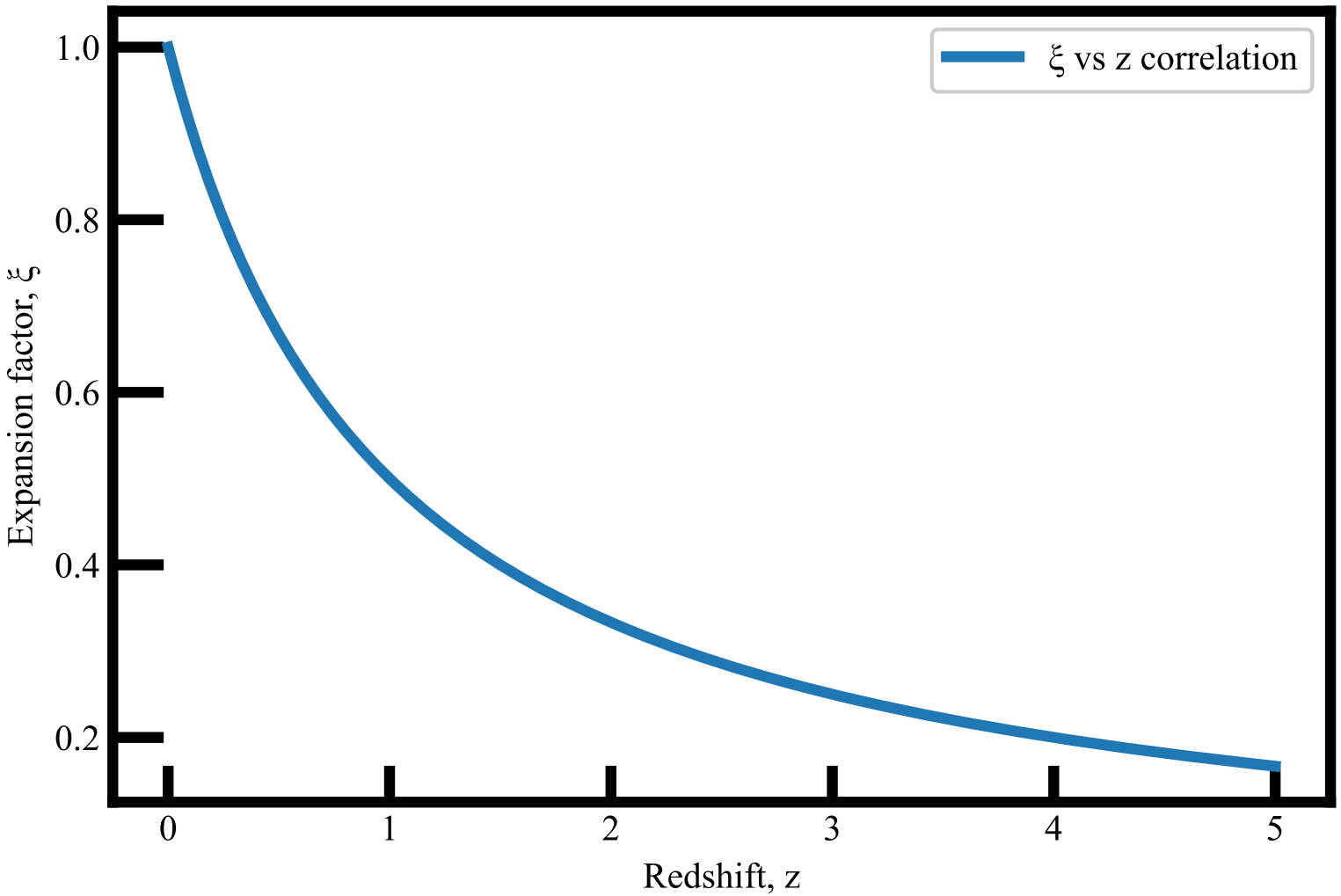
Plotting our present & future
The *arctanh* and *magarctanh* models





The calculated curve on the *mag*arctanh model approaches 0,0 but Python returns an error message for a value of *mag* at z=0.

Plotting transformed metric
The ξ vs z relationship



This trace of the expansion factor, ξ, vs redshift, z, displays a nonlinear relationship.

Notes on terms
Some terms applied to spacetime geometry

The following terms are used interchangeably by many physicists though the exact meanings are not identical

- concave geometry and closed universe
- flat geometry and Euclidean and quasi-Euclidean geometry
- convex geometry and open universe*
- *convex geometry is impossible in a universe with matter - possible only in a universe with anti-gravity