Class overview today - March 21, 2016

- **Part I - Common statistical methods in geoscience**
  - The many challenges of **geological data samples**
  - **Uncertainty** in Earth science data
  - Basic mathematical representations of **measurement uncertainty**
- **Part II - What do geochronological ages mean?**
  - **Geochronological ages and their meaning**
  - **Comparing** predicted and measured ages
  - **Quantifying the fit** of predicted and measured ages

Introduction to Quantitative Geology
Lecture 4
What do geochronological ages mean?

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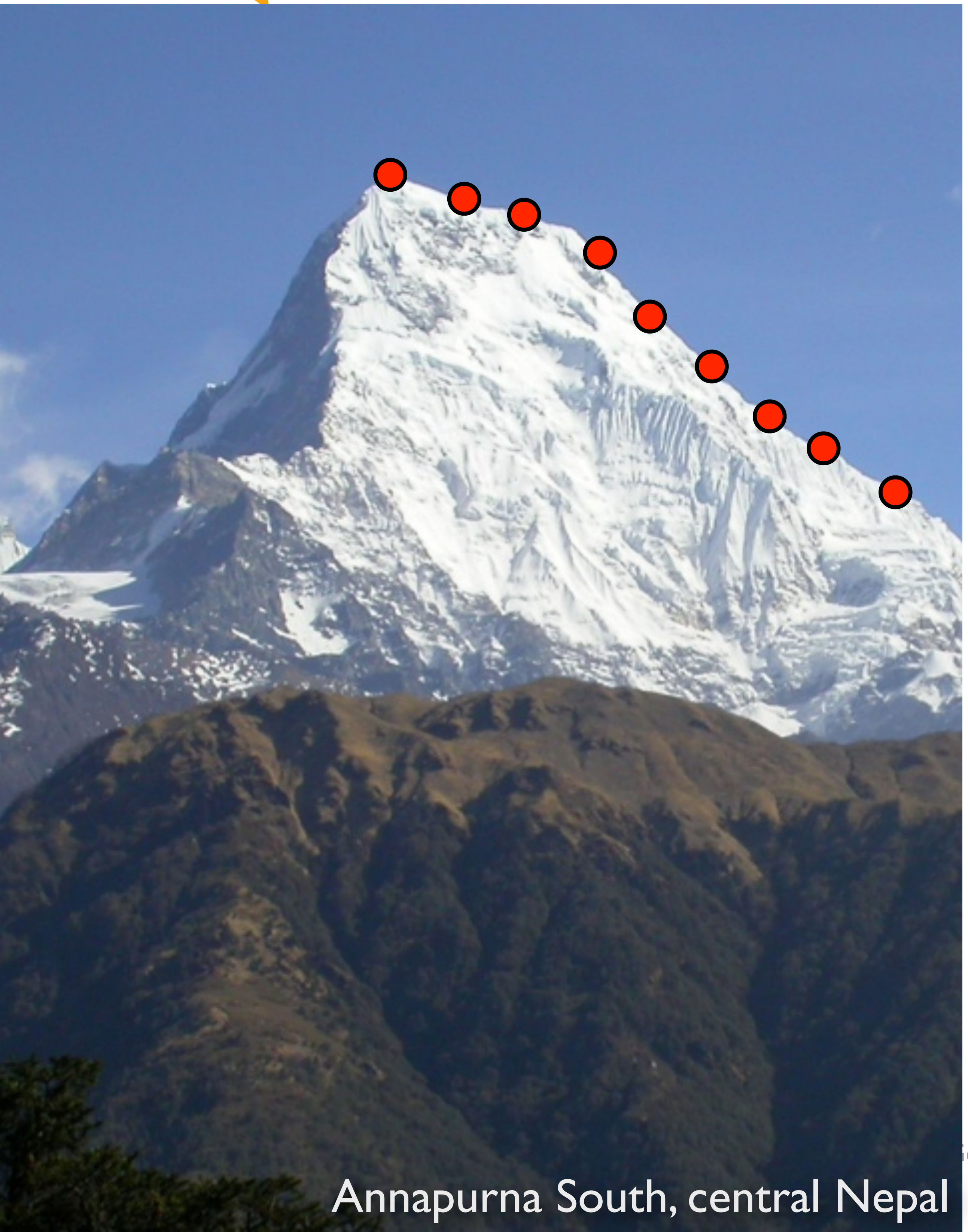
Goals of this lecture

- Provide an overview of **geochronological ages and their meaning**
- Discuss how to **compare** predicted and measured ages
- Introduce the basic concepts of **quantifying the fit** of predicted and measured ages

Geochronological ages



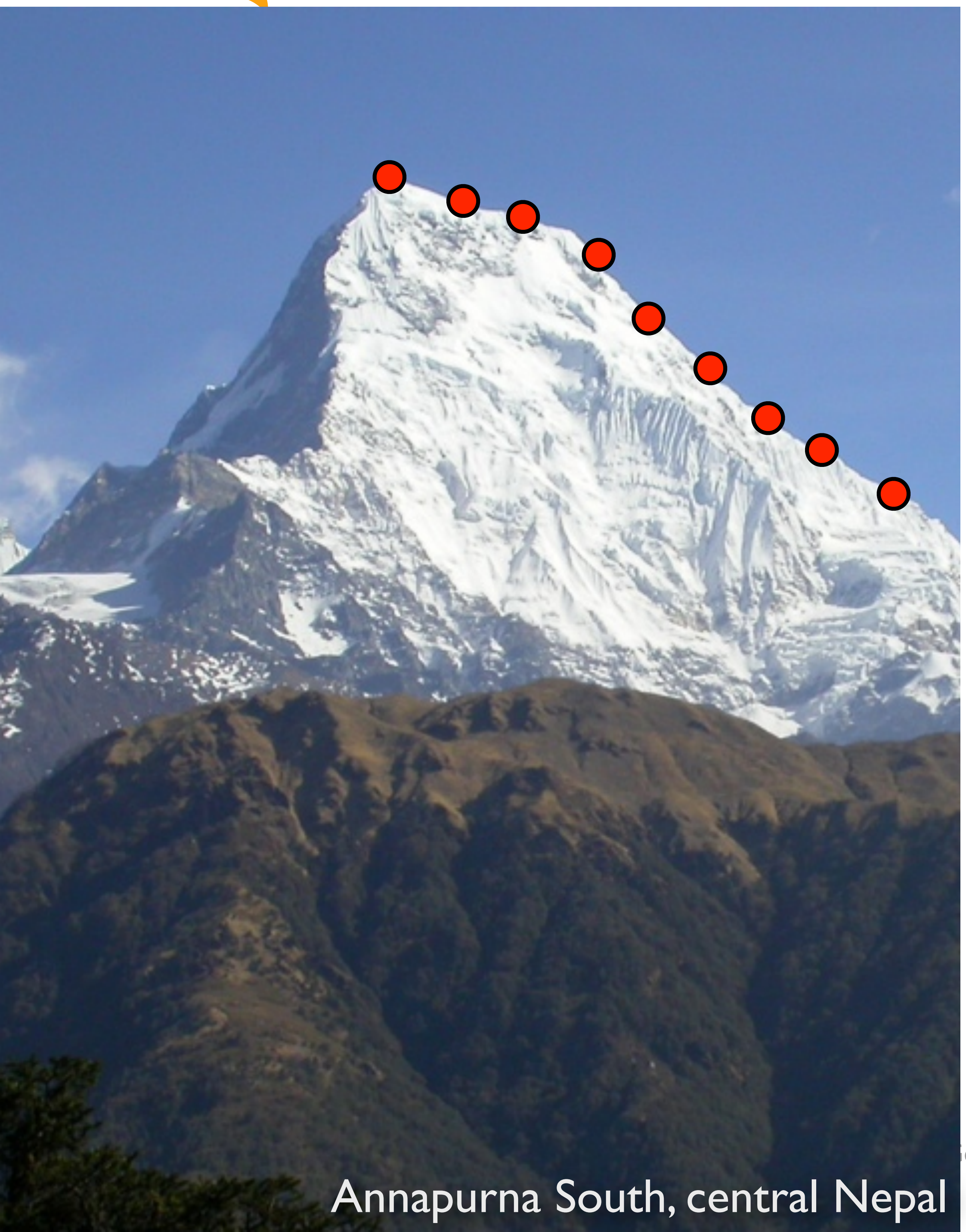
Annapurna South, central Nepal

- **Geochronology** is the science of determining the <u>age of geological features</u>

- Many methods are based on <u>radioactive decay of parent isotopes and measurement of accumulation of daughter isotopes in a host mineral</u>

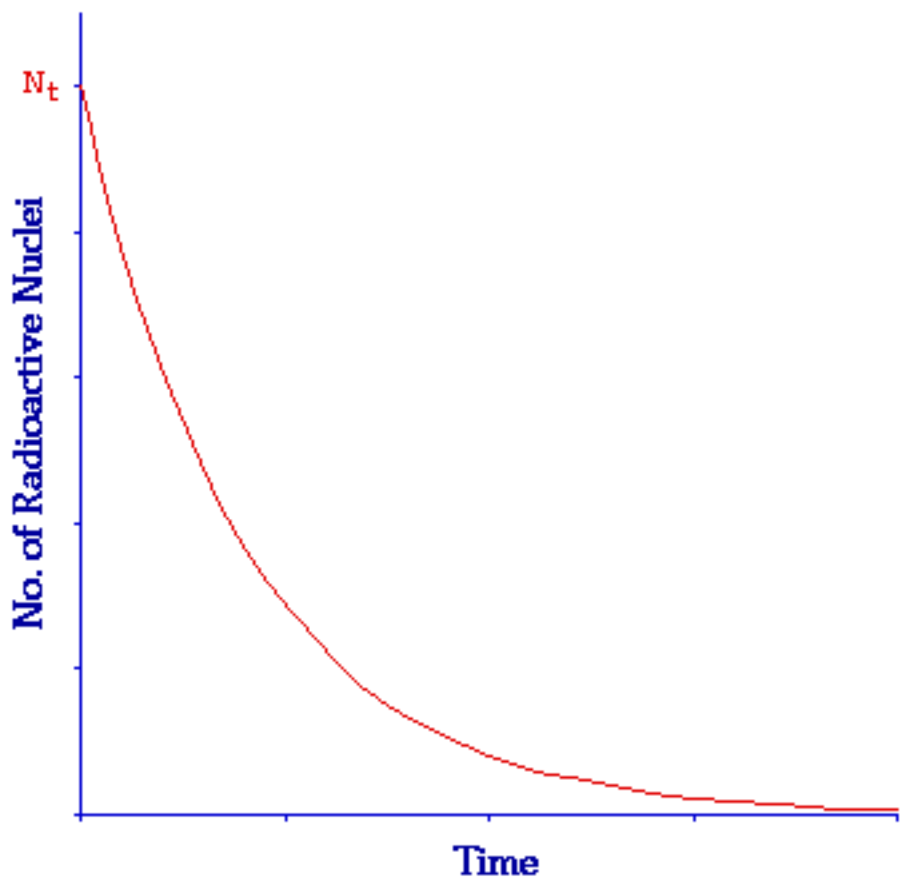
- As you might imagine, well-planned sample collection and minimising uncertainties is **critical**

Dating bedrock


Annapurna South, central Nepal

- Typical sample collection involves collection of several kg of bedrock, crushing, separation and dating of individual (or groups) of a specific mineral grain
- The resulting age calculation provides an <u>age for a specific sampled location</u>

Radioactive dating in a nutshell



- Many geological dating techniques rely on **radioactive decay** to determine geological age
- The rate of **radioactive decay** of parent isotope is proportional to the concentration of the parent isotope N

$$\frac{dN}{dt} = -\lambda N$$

  - The proportionality constant λ is called the **decay constant** and has units of $1/\mathrm{time}$

- The solution to this equation has the form

$$N(t) = N_0 e^{-\lambda t}$$

where N_0 is the initial parent isotope concentration

Radioactive dating in a nutshell

- If none of the daughter product D has been lost, the initial concentration of the parent isotope is simply

$$N_0 = N + D$$

- Thus, the parent isotope concentration

$$N(t) = N_0 e^{-\lambda t}$$

can be written as

$$N(t) = N = (N + D)e^{-\lambda t}$$

Radioactive dating in a nutshell

$$N(t) = N = (N + D)e^{-\lambda t}$$

- To find the geochronological age based on radioactive decay, we simply solve for t

$$N = (N + D)e^{-\lambda t}$$

$$Ne^{\lambda t} = N + D$$

$$e^{\lambda t} = \frac{N + D}{N}$$

$$e^{\lambda t} = 1 + \frac{D}{N}$$

$$\lambda t = \ln\left(1 + \frac{D}{N}\right)$$

$$\boxed{t = \frac{1}{\lambda}\ln\left(1 + \frac{D}{N}\right)}$$

Common half-lives

Parent isotope	Daughter isotope	Half-life $t_{1/2}$ [Ga]
^{40}K	^{40}Ar	1.25
^{232}Th	^{208}Pb	14
^{235}U	^{207}Pb	0.704
^{238}U	^{206}Pb	4.47

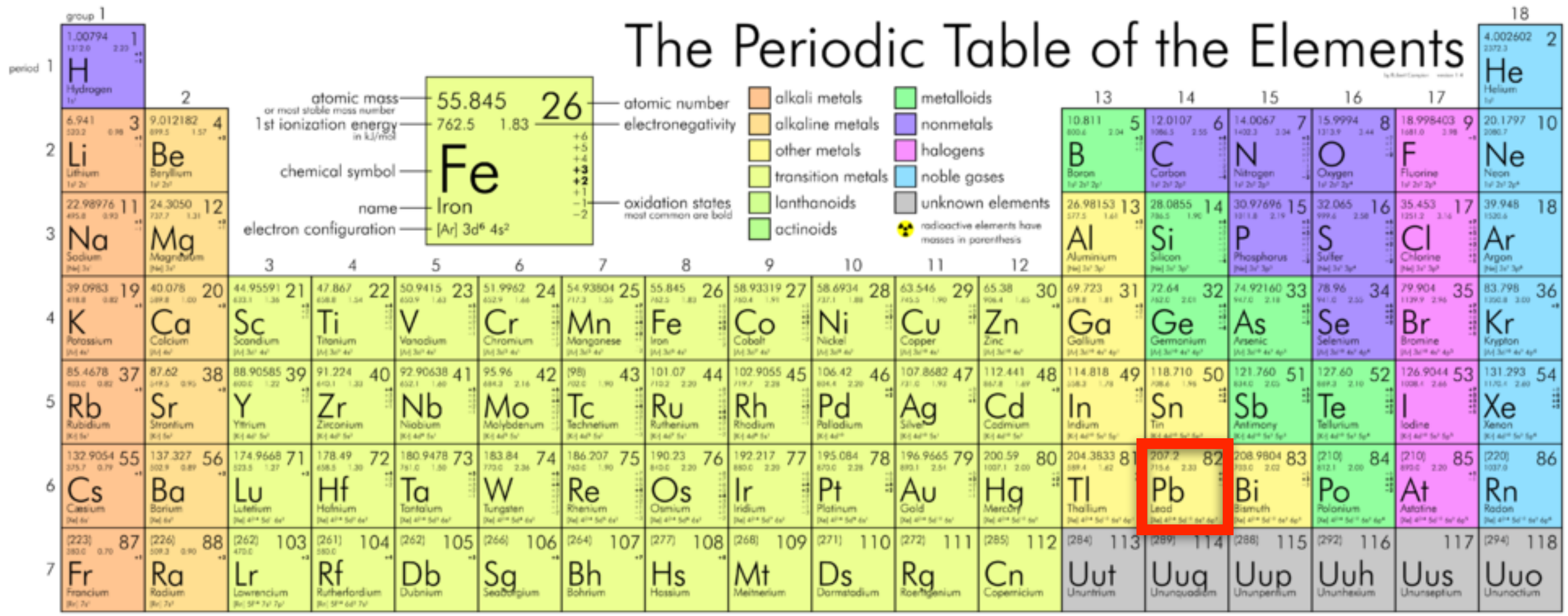
- The **half-life** of a radioactive material is the <u>time needed for half of the parent isotope to decay</u>

Common half-lives

Parent isotope	Daughter isotope	Half-life $t_{1/2}$ [Ga]	Decay constant λ [10^{-11} a^{-1}]
^{40}K	^{40}Ar	1.25	5.81
^{232}Th	^{208}Pb	14	4.948
^{235}U	^{207}Pb	0.704	98.485
^{238}U	^{206}Pb	4.47	15.5125

- The **half-life** of a radioactive material is the time needed for half of the parent isotope to decay
- Half-life $t_{1/2}$ is related to the decay constant λ: $t_{1/2} = \frac{ln(2)}{\lambda}$
- The radioactive isotopes above are commonly used in geology
  - The listed daughter product is *one* of the stable daughters
- Half-life uncertainties are generally quite small (<0.5%)

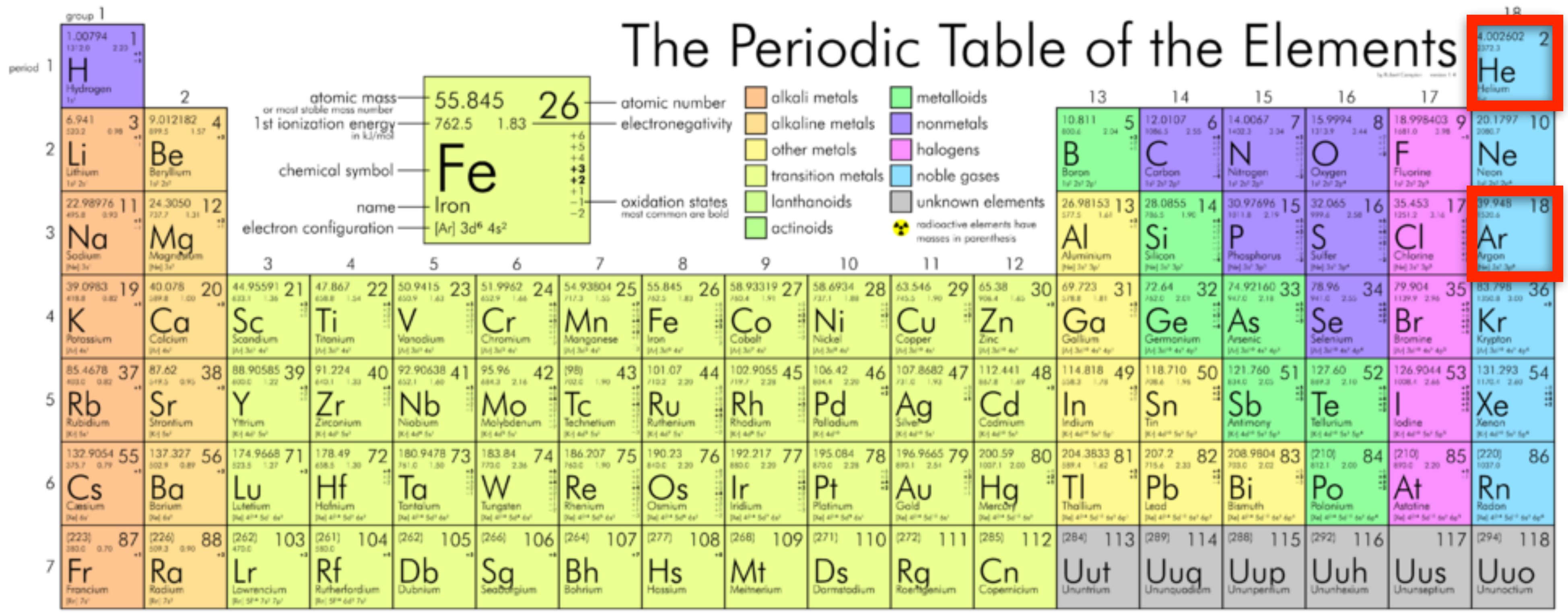
Crystallisation versus cooling ages



Lathanide and actinide series not shown

- In general, a good geochronometer is one with concentrations of isotopes that are <u>easily measured</u> and a <u>daughter product that is retained in the crystal</u>
  - Lead isotopes are a nice example of effectively 'immobile' daughter products
    - U-(Th)-Pb dating in zircons is widespread and useful
  - The age measured by mineral geochronometers can be considered a crystallisation (or formation) age

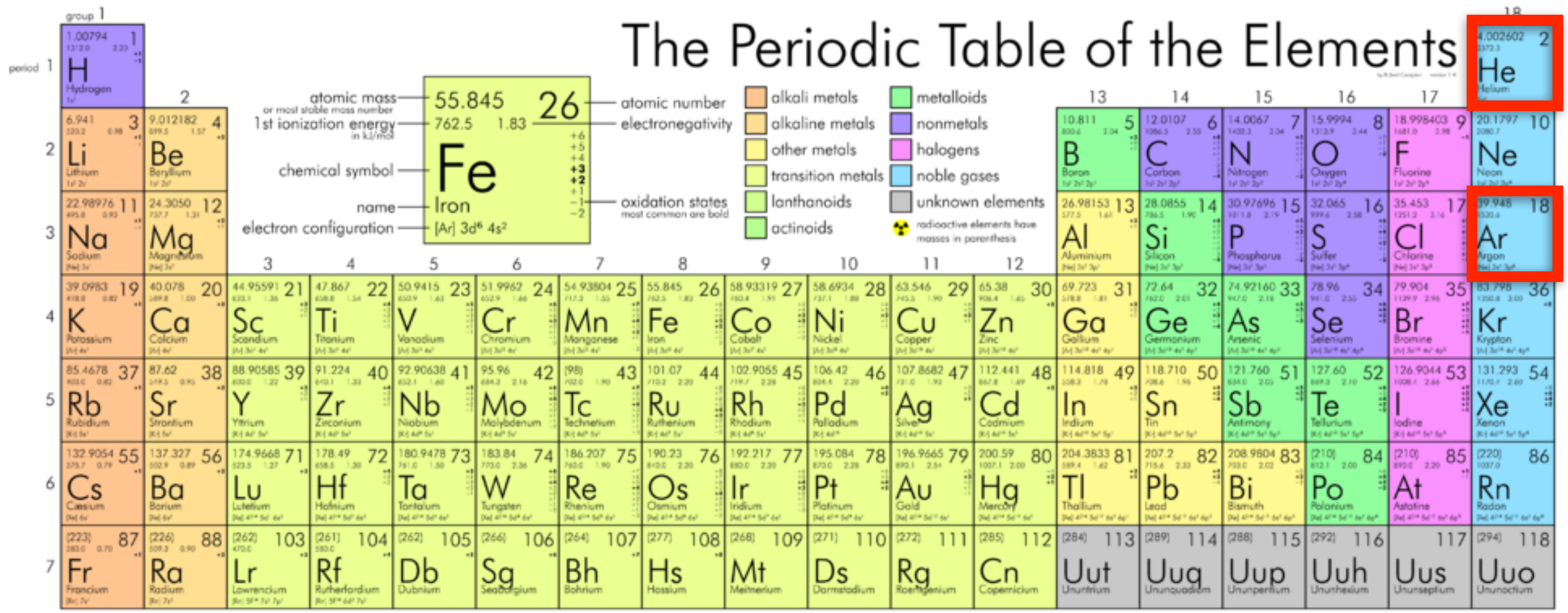
Crystallisation versus cooling ages



Lathanide and actinide series not shown

- Some radioactive daughter products are <u>mobile and can diffuse within the host crystal</u>, and thus <u>their concentration in the mineral may not record a crystallisation age</u>
- Temperature is one of the main influences on the rate of daughter product diffusion, and the daughter product is effectively not lost by solid-state diffusion when the mineral of interest is below its "closure temperature"
- These "**cooling ages**" are the basis of **thermochronology**

Crystallisation versus cooling ages



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- For example, ^{4}He is produced by decay of ^{238}U, ^{235}U and ^{232}Th, which are often present in the mineral zircon in minor concentrations
- ^{4}He is only retained within zircon crystals over geological time at temperatures below ~180°C
- This behaviour is the basis for zircon (U-Th)/He thermochronology

Major point 1: What does your age record?

- As you can see, depending on the chosen dating system, your chronometer may record different things:
  Crystallisation or cooling

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- Plutons can take millions of years to cool. **How might the zircon U-Pb and (U-Th)/He ages compare for a large pluton?**

Major point 1: What does your age record?

- As you can see, depending on the chosen dating system, your chronometer may record different things:
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- Plutons can take millions of years to cool. **How might the zircon U-Pb and (U-Th)/He ages compare for a large pluton?**
- **What about a 0.5 m-wide dike?**

Uncertainties in geochronological data

Coutand et al., 2014

Samples	^{238}U (mol)	^{232}Th (mol)	^{147}Sm (mol)	^{4}He (mol)	Mean L (µm)	Mean R (µm)	Raw Age (Ma)	Ft	Corrected Age (Ma)	Age Error (%)	Mean Age (Ma)	Error (Ma)
BH63-1	9.55E-13	2.53E-13	4.81E-12	5.30E-15	253	79.5	3.96	0.83	4.77	2.00	4.2	0.4
BH63-2	1.38E-12	3.08E-13	3.18E-12	7.59E-15	269	59.5	4.02	0.79	5.11	1.93		
BH63-3	6.65E-13	1.52E-13	2.29E-12	2.34E-15	206	57.5	2.55	0.77	3.30	2.17		
BH63-4	9.39E-13	2.12E-13	3.51E-12	3.47E-15	248	65.5	2.67	0.80	3.34	2.07		
BH63-5	1.27E-12	4.04E-13	3.23E-12	6.19E-15	226	60	3.48	0.78	4.45	1.96		

[a]Abbreviations: L, grain length; R, grain radius; Ft, alpha-ejection correction factor. Mean ages are the mean of each selected aliquot and the age error is the standard deviation between selected aliquots divided by the square root of the number of aliquots.

- Typical uncertainties in geochronological ages include:
  - Measurement uncertainty
    - Uncertainty based on the ability to measure the isotopes (or features) of interest precisely
  - Decay constant uncertainty
  - "Geological complexity" uncertainty
    - **Difficult to quantify and common :(**

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Typically small

- Measurement uncertainty
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Can be large

- "Geological complexity" uncertainty
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A typical age measurement

- Reported geochronological ages are often the mean age of several replicate age determinations for each sampled location
  - Ages are typically calculated for 5 or more individual mineral grains from a single collected sample
    - The uncertainty in these grain ages would be related to the **measurement uncertainty** and **uncertainty in the constants**, such as the decay constant
  - **Mean ages** are calculated using the standard equation (see Lecture 3), or **weighted mean ages** are determined by

$$\bar{x} = \frac{\Sigma w_i x_i}{\Sigma w_i} \quad \text{where} \quad w = \frac{1}{\sigma_x^2}$$

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What is the potential advantage of calculating weighted mean ages?

Reported age uncertainty

- With our best estimate of a sample's age x_{best} based on the mean or weighted mean age, the standard deviation is one possible option to report uncertainty

- Often, the **standard deviation of the mean** $\sigma_{\bar{x}}$ is reported instead

$$\sigma_{\bar{x}} = \frac{\sigma_x}{\sqrt{N}}$$ (Also known as standard error)

- Thus, the reported **measured age** would be in the form

$$\text{Age} = x_{\text{best}} \pm \delta x$$

where $\delta x = \sigma_{\bar{x}} = \sigma_x / \sqrt{N}$

Standard deviation versus standard error

- How are they different, and what should you use?
  - **Standard deviation** is a measure of <u>how widely scattered measurements are from the mean</u>
    - Should not change with increasing sample size
  - **Standard error** is a measure of <u>uncertainty about the estimate of the sample mean</u>
    - Decreases with increasing sample size
- Where possible, <u>standard error is preferable</u>
- **Note**: When you list an age with its uncertainty, you should be clear whether the uncertainty is the standard deviation, standard error or something else

"Geological complexity"

- <u>Uncertainty based on the standard deviation or standard error reflects variations in individual mineral grain ages</u>, and is typically considerably larger than the uncertainty of the measurement of the individual grain ages

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"Geological complexity"

- Uncertainty based on the standard deviation or standard error reflects variations in individual mineral grain ages, and is typically considerably larger than the uncertainty of the measurement of the individual grain ages
    - **What could cause ages in a sample to vary?**

- This can be quite difficult to answer (and even harder to address), but common sources of variability in replicate grain age measurements include zoning of the parent isotope(s), partial loss of daughter products, radioactive mineral inclusions, inherited daughter products (such as in old mineral cores), poor mineral morphology, …

Comparing model predictions to age data

Part of the point of a course like this is to learn to use mathematical models to make geological predictions

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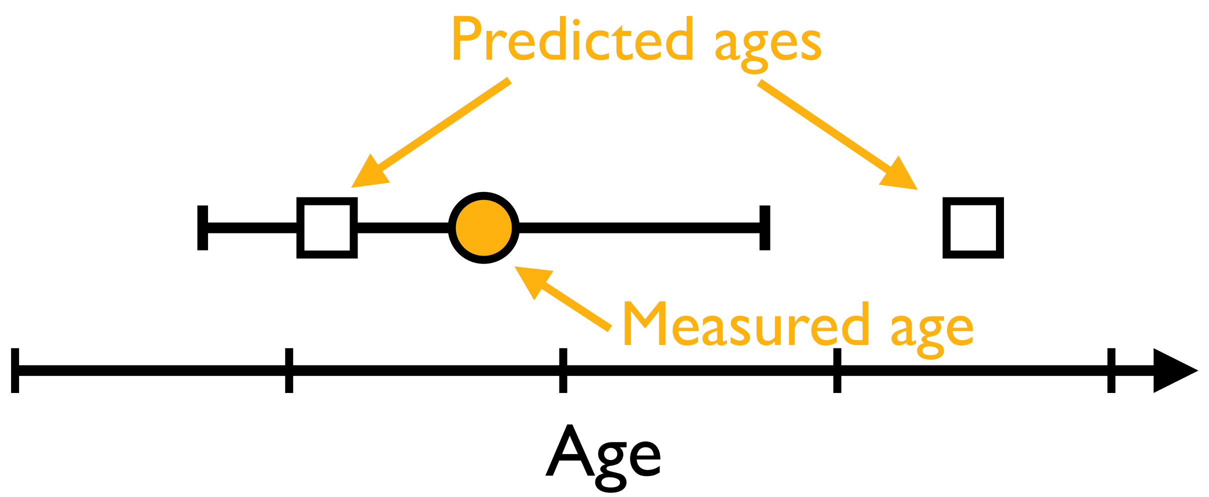
- How do we compare measured and predicted ages, taking care to consider the age uncertainties?
- When can we consider a predicted age to be equal to a measured age?

Comparing model predictions to age data



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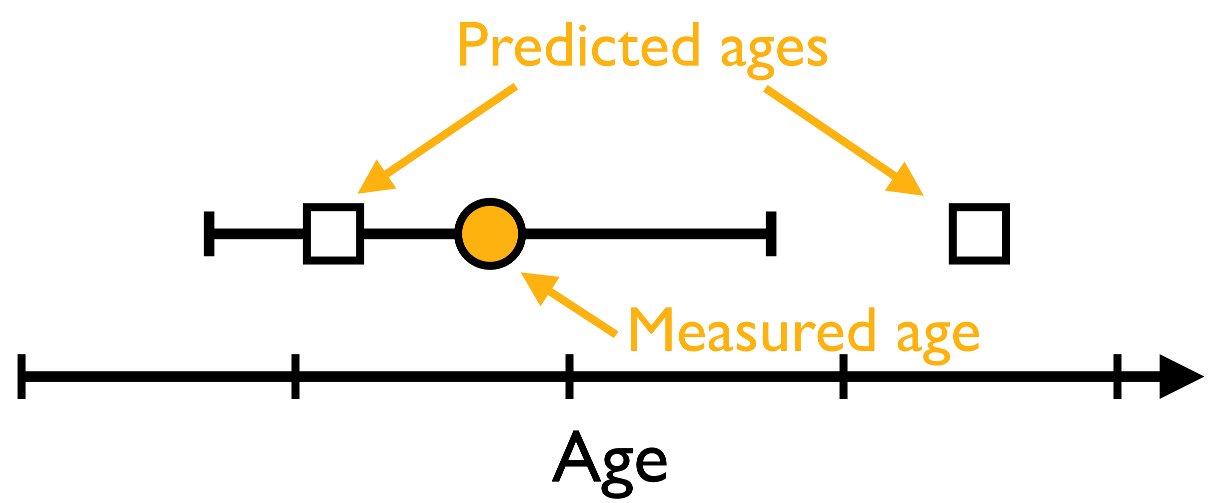
Major point II:
Predicted ages must be within uncertainty



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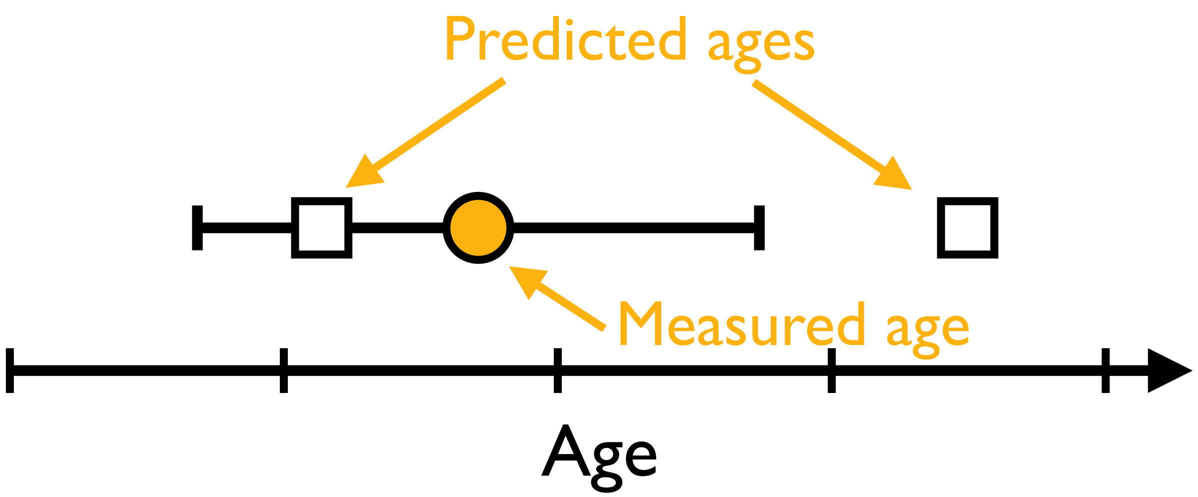
Goodness of fit

- Because we know the uncertainty of our measured ages, we can quantify how well a set of predicted ages "fit" our measured ages
- Equations of this type are known as **goodness of fit** statistics
- One basic **goodness of fit** statistic is the **weighted sum of the squared errors**

$$\chi^2 = \sum \frac{(O - E)^2}{\sigma^2}$$

where χ^2 is the goodness of fit, O is the observed age, E is the predicted age and σ is the standard deviation

Goodness of fit for a single age



$$\chi^2 = \sum \frac{(O - E)^2}{\sigma^2}$$

- What does the χ^2 value mean?
  - Let's consider two examples:
    - O_1: 5.4 ± 0.8 Ma
      E_1: 5.0 Ma
      χ^2: $(5.4 - 5.0)^2/0.8^2$ = **0.25**
    - O_2: 5.4 ± 0.8 Ma
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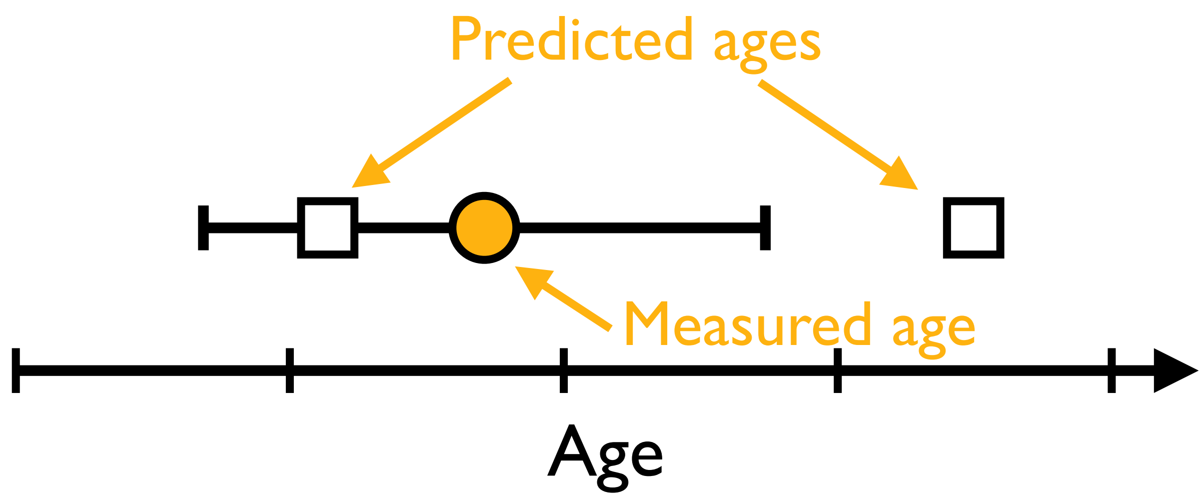
      χ^2: $(5.4 - 6.8)^2/0.8^2$ = **3.0625**

Goodness of fit for a single age



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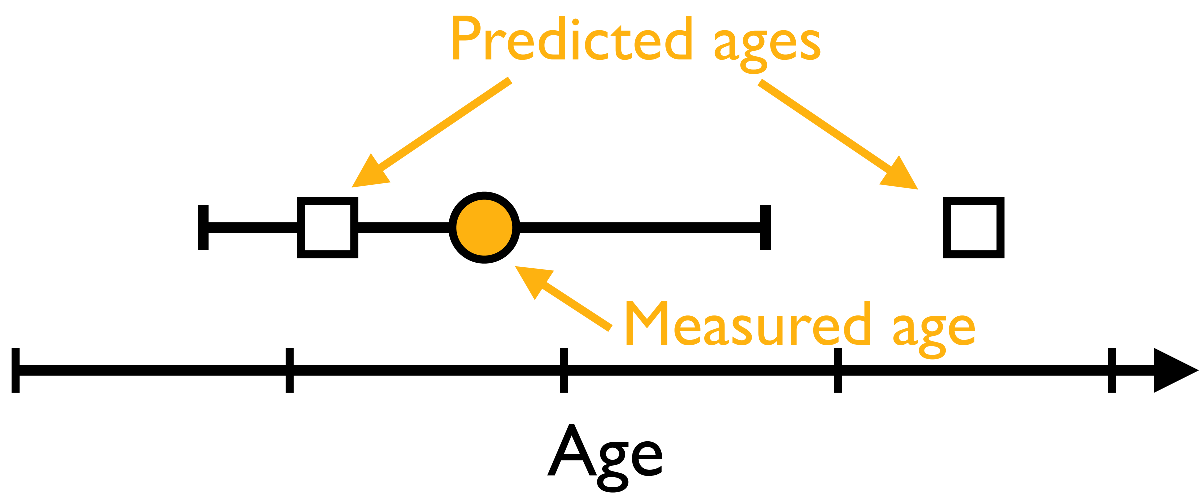
What does it mean when χ^2 = 1 for a single age?

Goodness of fit for a single age



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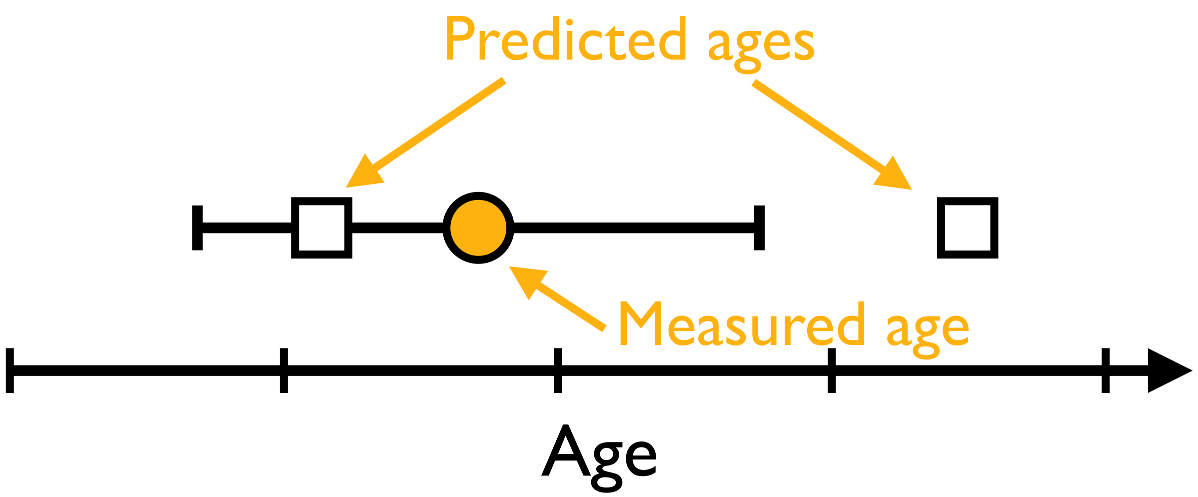
What does it mean when χ^2 = 1 for a single age?

$\chi^2 \leq 1$: Predicted age with measurement uncertainty (for a single measurement)

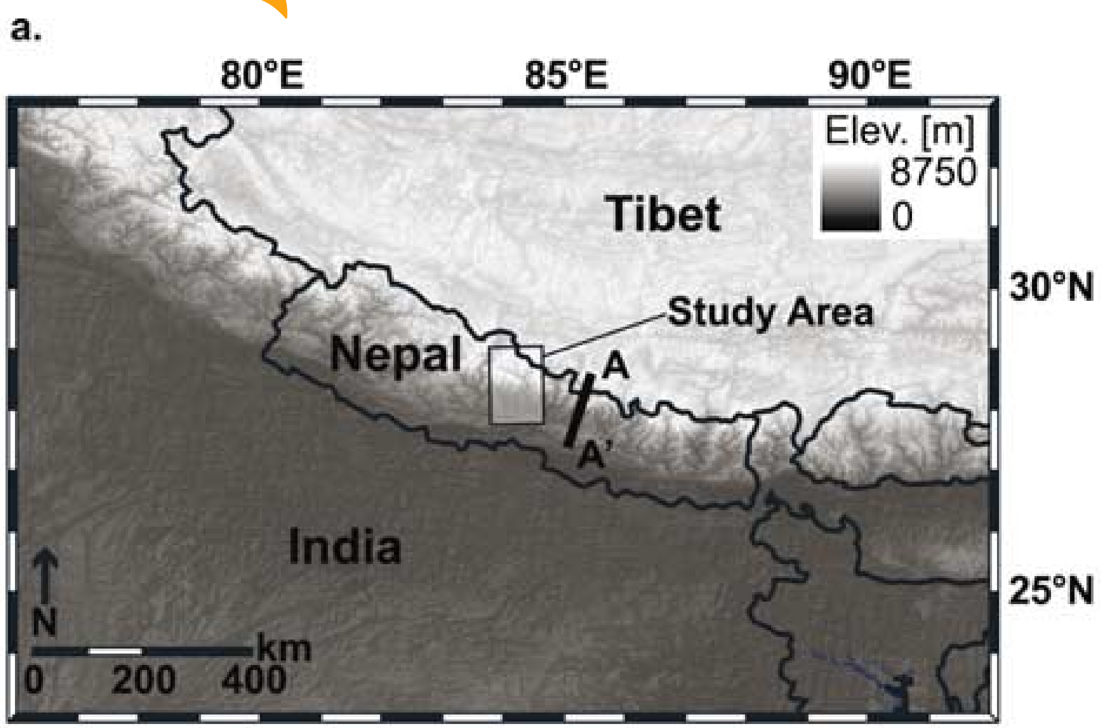
Goodness of fit for multiple ages

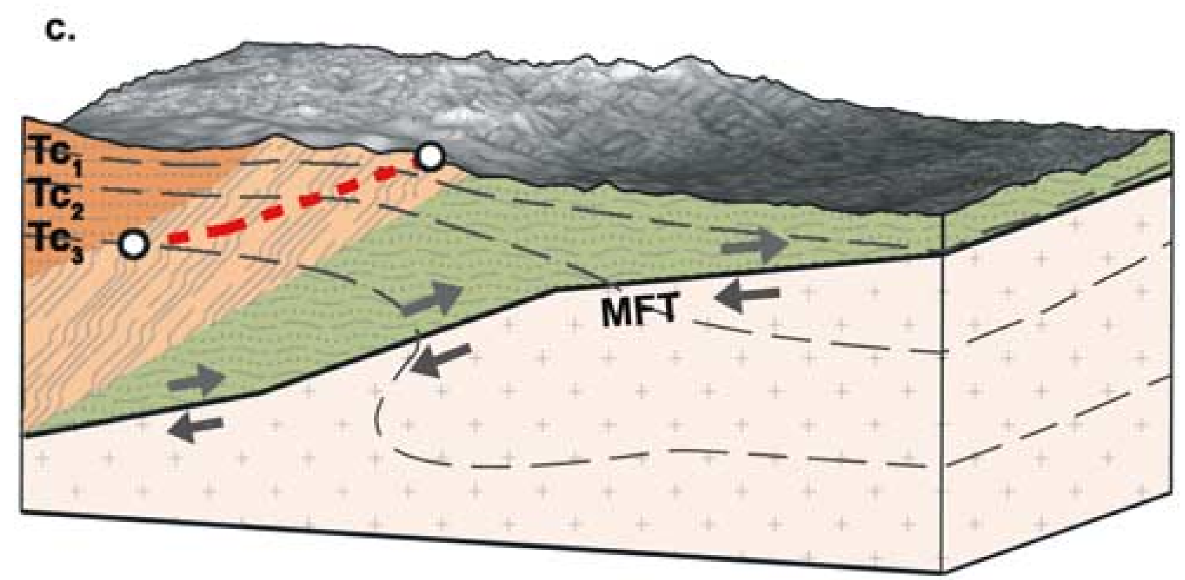


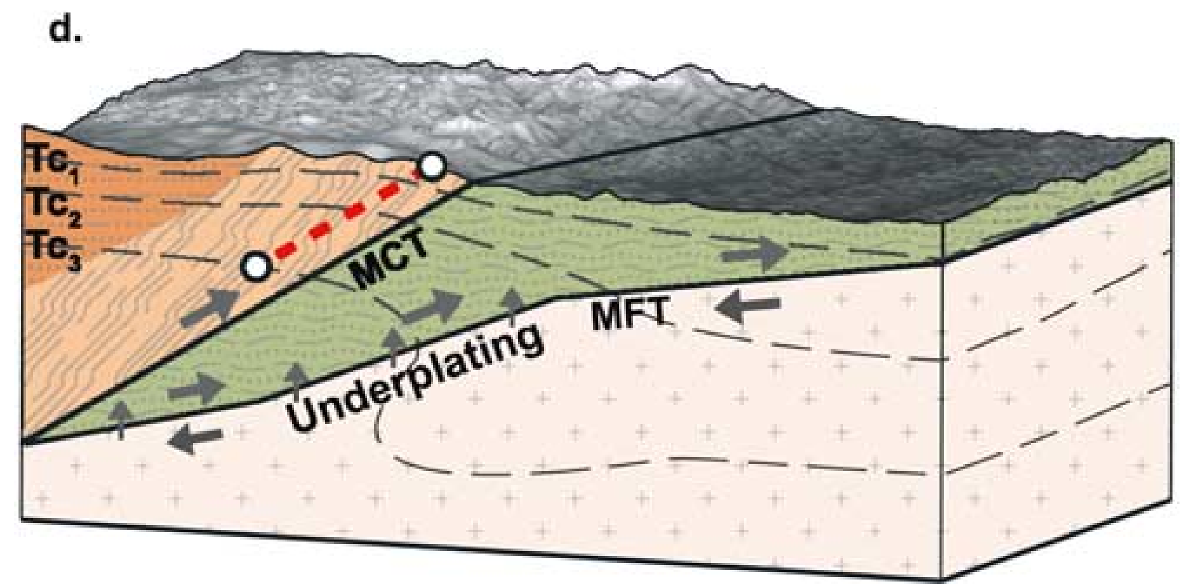
$$\chi^2 = \sum \frac{(O - E)^2}{\sigma^2}$$

- What does the χ^2 value mean?
  - If we calculate the χ^2 value for both ages together, the value is $\chi^2 = 0.25 + 3.0625 = \mathbf{3.3125}$
  - Although this value itself is less intuitive, it can be <u>compared to the chi-squared distribution to determine its meaning</u>
  - Alternative formulations can also be used, where, for example. the <u>number of measured ages</u> is considered in the goodness of fit

So…why is this useful?







Central Nepal Himalaya:
We used a numerical model to predict cooling ages from two hypothesized tectonic scenarios and compared them to observed ages

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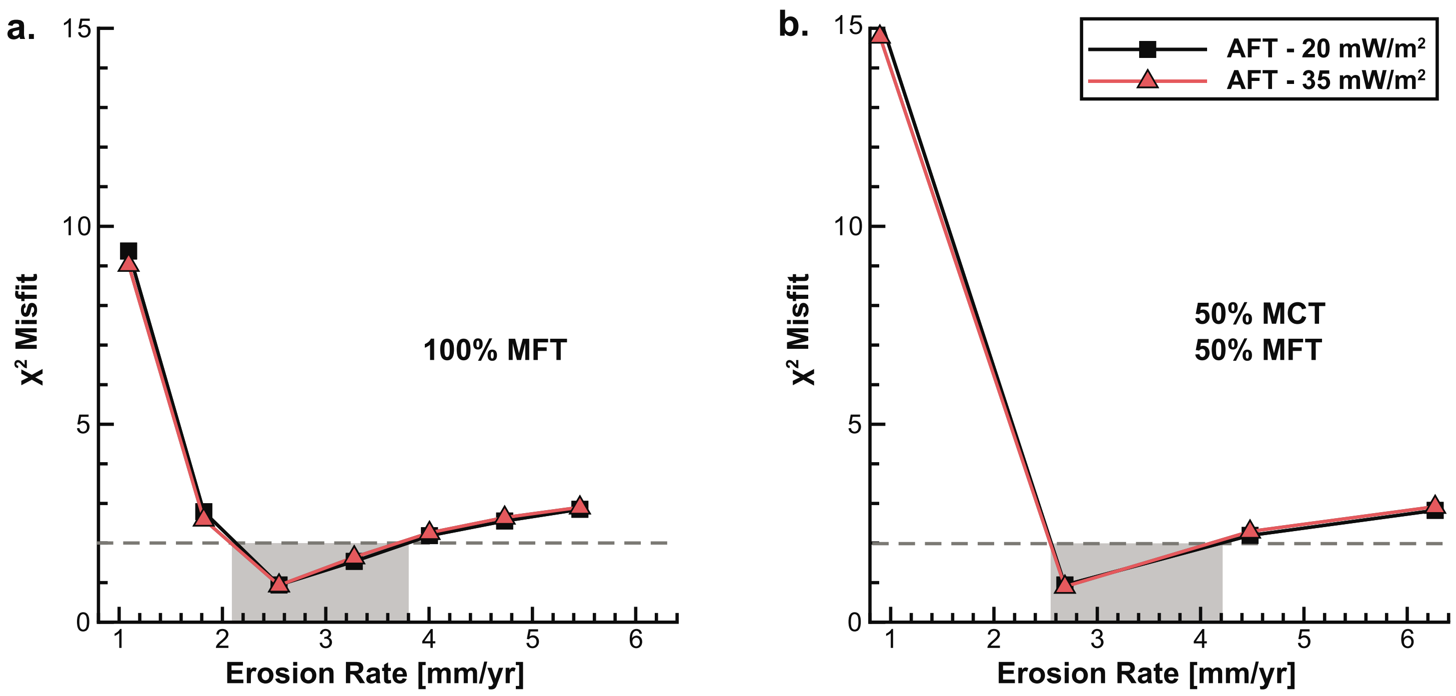

- Fault slip was partitioned onto two faults:
  - MFT - Main frontal thrust
  - MCT - Main central thrust

- Main finding:
  - Which fault was active has little influence on the ages as long as the rock uplift/ erosion rate is 2-5 mm/yr

Recap

- Why might the daughter isotope for a geochronometer matter when interpreting a geochronological age?
- How can we compare predicted and measured ages?
- The χ^2 value for 100 predicted and measured ages is exactly zero.
  - What does this mean?
  - Is it reasonable?

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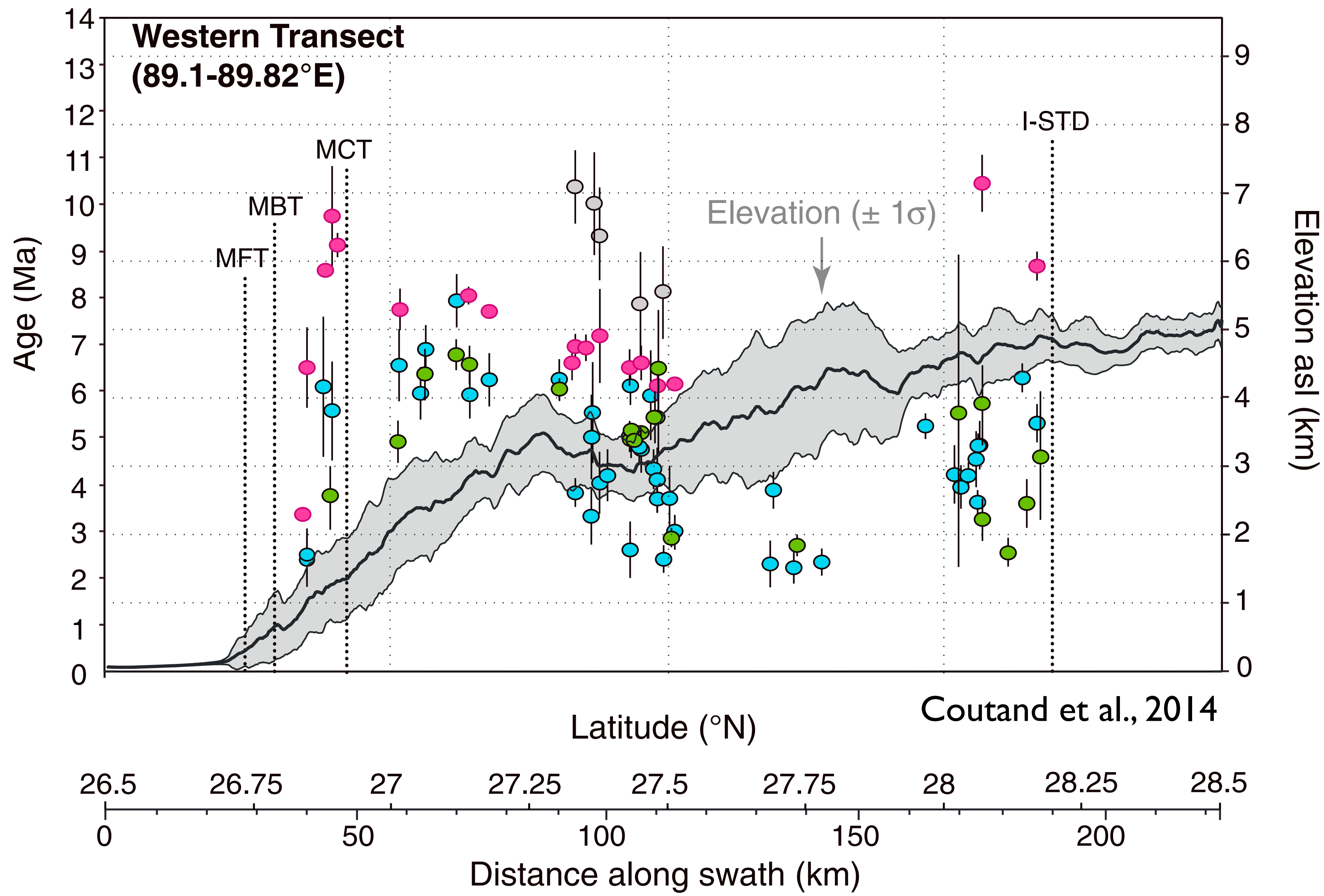
Lab preview



- This week we will continue developing our Python skills by **plotting** and **interpreting** geochronological data

References

Coutand, I., Whipp, D. M., Grujic, D., Bernet, M., Fellin, M. G., Bookhagen, B., et al. (2014). Geometry and kinematics of the Main Himalayan Thrust and Neogene crustal exhumation in the Bhutanese Himalaya derived from inversion of multithermochronologic data. *Journal of Geophysical Research: Solid Earth*, n/a–n/a. doi:10.1002/2013JB010891