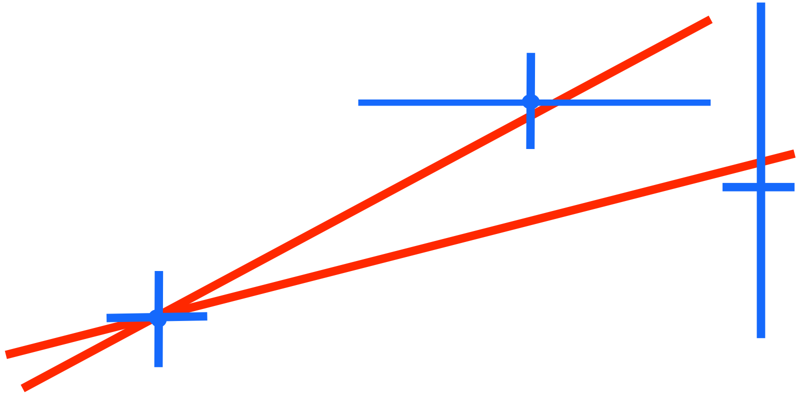
Error Bars in both X and Y



Wrong ways to fit a line :

1. $y(x) = a\,x + b \quad (\sigma_x = 0)$

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Example: Primordial He abundance:

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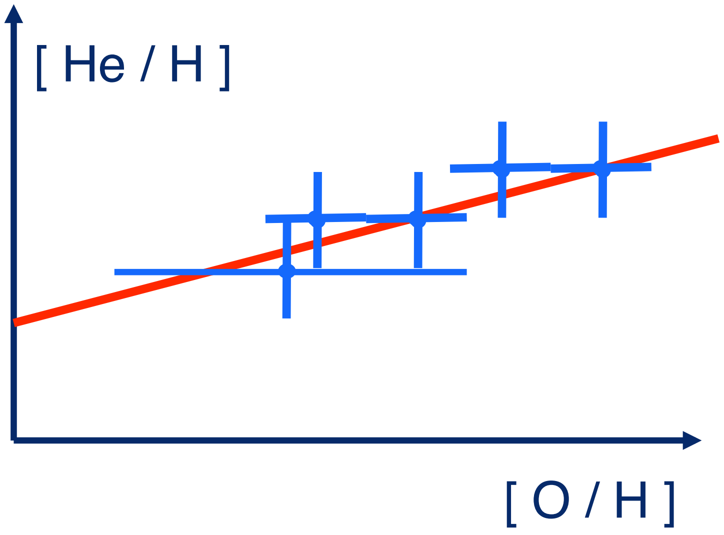


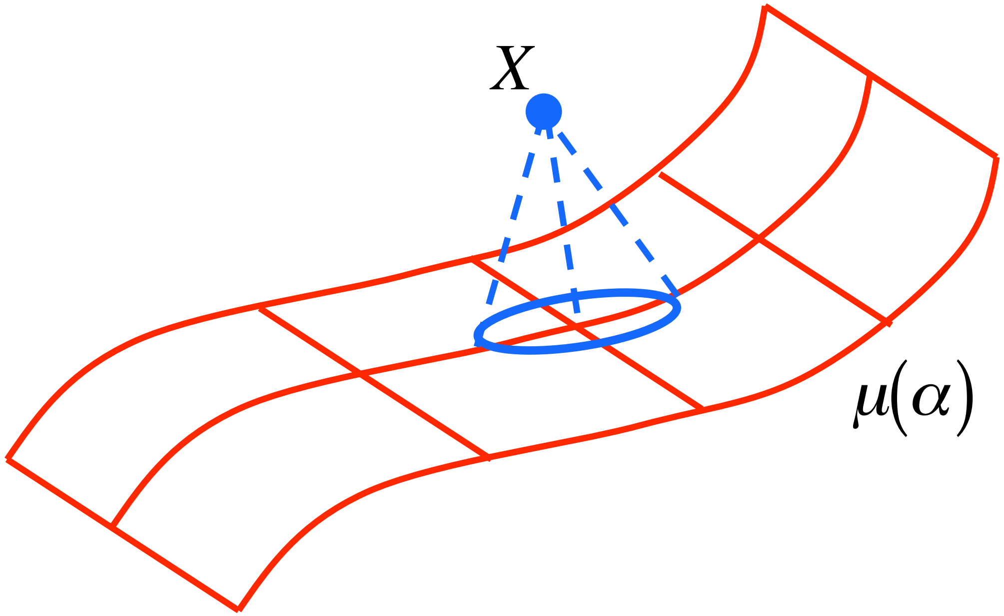
Vector Space Perspective

N data points, M parameters.

Model $\mu(\alpha)$ defines a parameterised M-dimensional surface in the N-dimensional data space.

$\chi^2(\alpha)$ = squared distance from the observed data to the model surface.

Best-fit model is the one closest to the data.



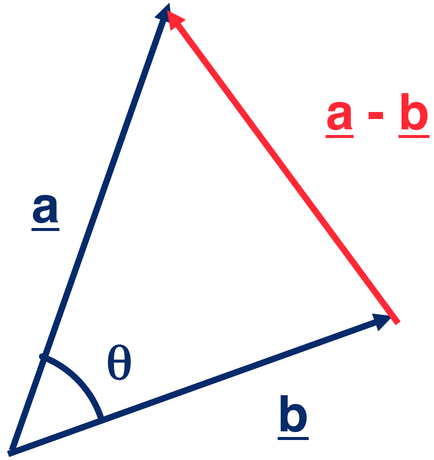
For linear models (scaling patterns), the model surface is a flat M-dimensional hyper-plane.

Review: Vector spaces

Dot product:

$$\underline{\mathbf{a}} \bullet \underline{\mathbf{b}} = |\underline{\mathbf{a}}||\underline{\mathbf{b}}|\cos\theta$$

$$\theta = \text{"angle" between vectors } \underline{\mathbf{a}},\ \underline{\mathbf{b}}.$$



Length of a vector:

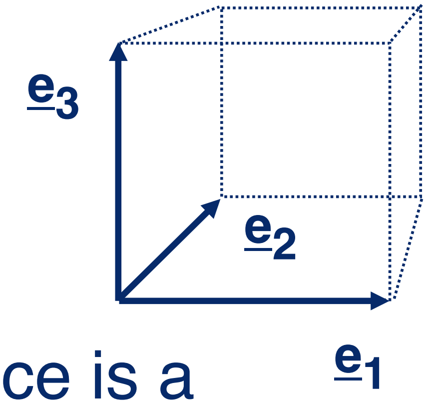
$$|\underline{\mathbf{a}}|^2 \equiv \underline{\mathbf{a}} \bullet \underline{\mathbf{a}}$$

(distance of point **a** from origin)

Distance between 2 vectors **a**, **b**

$$|\underline{\mathbf{a}} - \underline{\mathbf{b}}|$$

Ortho-normal Basis Vectors



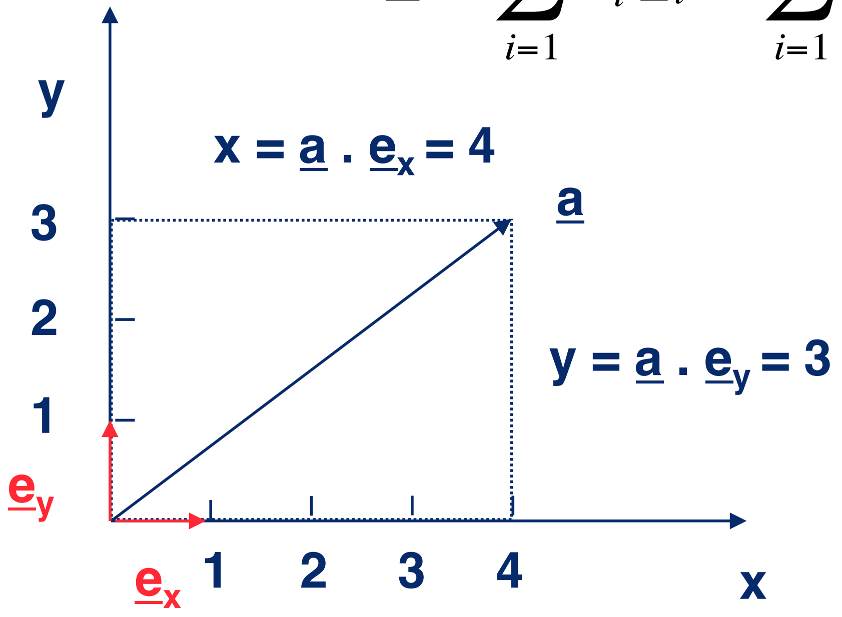
Ortho-normal basis vectors $\underline{e}_i$:

$$\underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

Any vector $\underline{a}$ in the *N*-dimensional vector space is a linear combination of the *N* basis vectors $\underline{e}_i$, with scale factors a_i

$$\underline{\mathbf{a}} = \sum_{i=1}^{N} a_i \, \underline{\mathbf{e}}_i = \sum_{i=1}^{N} \left(\underline{\mathbf{a}} \bullet \underline{\mathbf{e}}_i \right) \underline{\mathbf{e}}_i$$

Example:



Data Space is a Vector Space

N data points define a vector in *N*-dimensional "data space":

$$\underline{\mathbf{x}} = \{x_1, x_2, \ldots, x_N\}$$

$$= x_1\,\underline{\mathbf{e}}_1 + x_2\,\underline{\mathbf{e}}_2 + \ldots + x_N\,\underline{\mathbf{e}}_N$$

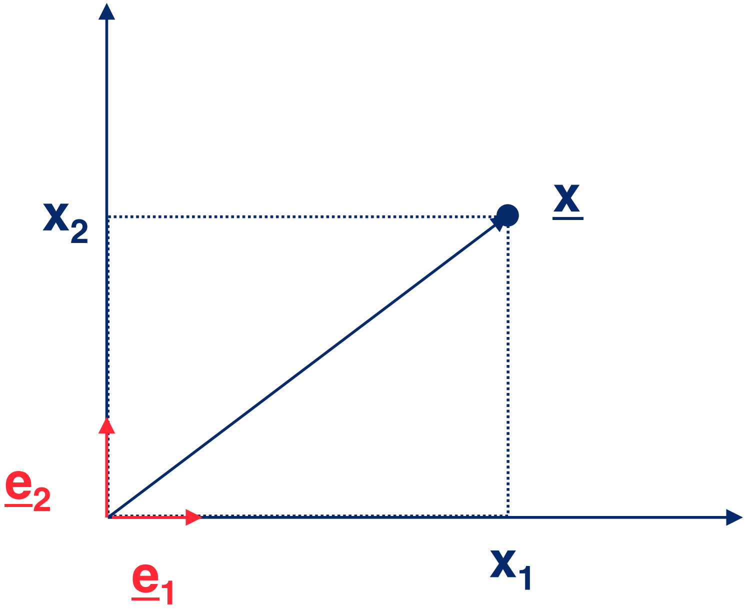
N basis vectors:

$$\underline{\mathbf{e}}_1 = \{1, 0, \ldots, 0\}$$

$$\underline{\mathbf{e}}_2 = \{0, 1, \ldots, 0\}$$

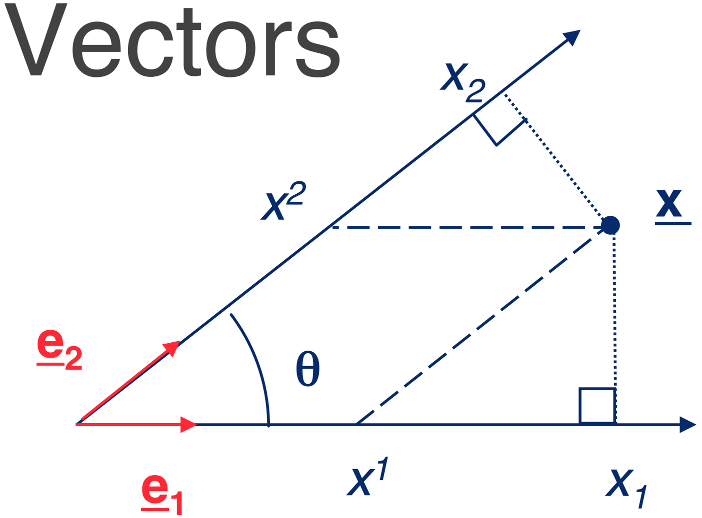
$$\ldots$$

$$\underline{\mathbf{e}}_N = \{0, 0, \ldots, 1\}$$



- Basis is ortho-normal if: $\underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j = \delta_{ij}$
- Basis vector $\underline{\boldsymbol{e}}_i$ selects data point x_i: $\underline{\mathbf{x}} \bullet \underline{\mathbf{e}}_i = x_i$
- Data point x_i is the projection of data vector $\underline{\mathbf{x}}$ along the basis vector $\underline{\boldsymbol{e}}_i$.

Non-orthogonal Basis Vectors



In the non-orthogonal case, $\underline{\mathbf{e}}_1 \bullet \underline{\mathbf{e}}_2 = \cos\theta \neq 0$

Two ways to measure coordinates:

- **contravariant** coordinates (index high)**:**

  x^i project **parallel** to basis vectors:

$$\underline{\mathbf{x}} = x^1 \underline{\mathbf{e}}_1 + x^2 \underline{\mathbf{e}}_2 + \ldots + x^N \underline{\mathbf{e}}_N$$

- **covariant** coordinates (index low):

  x_i project **perpendicular** to basis vectors.

$$x_i = \sum_j g_{ij}\, x^j$$

- **metric tensor**: $g_{ij} \equiv \underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j$

$$x_1 = x^1 + x^2 \cos\theta$$

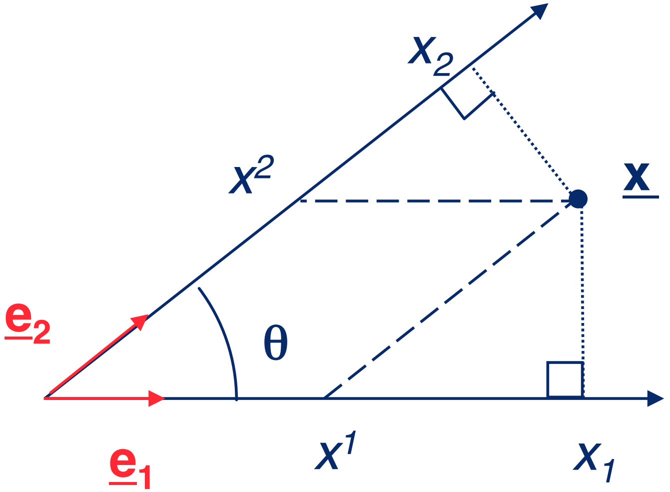
$$x_2 = x^2 + x^1 \cos\theta$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & \cos\theta \\ \cos\theta & 1 \end{bmatrix} \begin{bmatrix} x^1 \\ x^2 \end{bmatrix}$$

Dot product:

$$\underline{\mathbf{x}} \bullet \underline{\mathbf{y}} = \sum_{i,j} x^i\, y^j\, \underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j = \sum_{i,j} x^i\, y^j\, g_{ij} = \sum_i x^i\, y_i = \sum_j x_j\, y^j$$

Metric for non-orthonormal Basis Vectors



$$g_{ij} \equiv \underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j = \begin{Bmatrix} |\underline{\mathbf{e}}_1|^2 & |\underline{\mathbf{e}}_1||\underline{\mathbf{e}}_2|\cos\theta \\ |\underline{\mathbf{e}}_1||\underline{\mathbf{e}}_2|\cos\theta & |\underline{\mathbf{e}}_2|^2 \end{Bmatrix}$$

Metric is symmetric: $g_{ij} = g_{ji}$.

Off-diagonal terms vanish if the basis vectors are orthogonal.

Diagonal terms define the lengths of the basis vectors.

Data sets and Functions as Vector Spaces

- A data set, X_i, $i = 1, ..., N$, is also an N-component vector $(X_1, X_2, ..., X_N)$, one dimension for each data point.
- The data vector represents a single point in the N-dimensional data space.

- A function, $f(t)$, is a vector in an infinite-dimensional vector space, one dimension for each value of t.
- The "dot product" between 2 functions depends on a **weighting function** *w(t):*

$$\langle f,g\rangle \equiv \int_{-\infty}^{\infty} f(t)\, g(t)\, w(t)\, dt$$

Weighting function

Each weighting function *w(t)* gives a different dot product, a different distance measure, a different vector space.

Which w(t) to use for data analysis?

χ^2 as (distance)^2 in function space

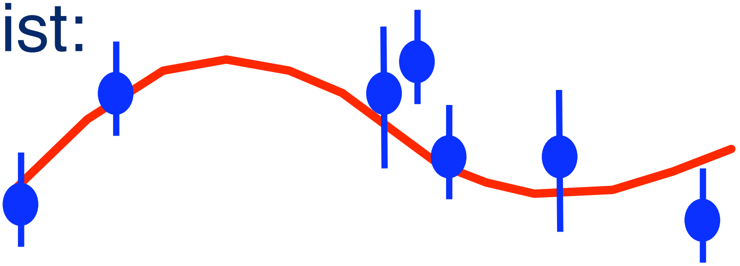
- The (absolute value)^2 of a function *f(t)* :

$$\| f \|^2 \equiv \langle f, f \rangle = \int f^2(t)\, w(t)\, dt$$

- The (distance)^2 between *f(t)* and *g(t)* :

$$\| f - g \|^2 \equiv \langle f - g, f - g \rangle = \int \left(f(t) - g(t) \right)^2 w(t)\, dt$$

- Define a weighting function *w(t)* that includes only the values at $t = t_i$, where data X_i exist:



$$w(t) \equiv \sum_{i=1}^{N} \frac{\delta(t - t_i)}{\sigma_i^2}$$

- Then the (distance)^2 from data to model is χ^2 :

$$\| X - \mu \|^2 = \sum_{i=1}^{N} \left(\frac{X_i - \mu(t_i)}{\sigma_i} \right)^2 = \chi^2 .$$

Each dataset has its own weighting function.

χ^2 as (distance)^2 in data space

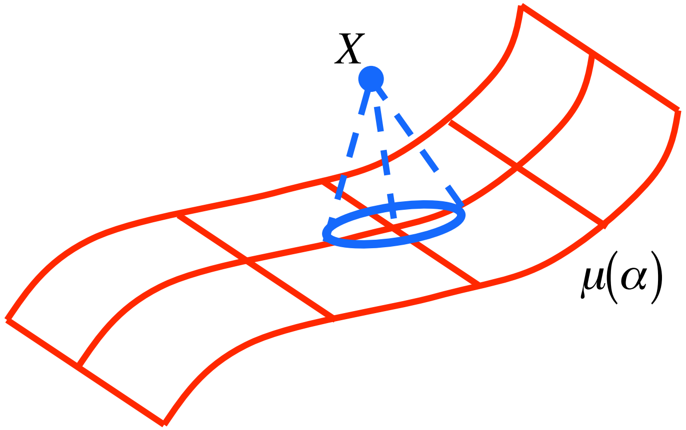
- In the data space, the dot product is defined with inverse-variance weights:

$$w_i = \frac{1}{\sigma_i^2} \quad \Rightarrow \quad \underline{\mathbf{a}} \bullet \underline{\mathbf{b}} = \sum_{i=1}^{N} a_i\, b_i\, w_i = \sum_{i=1}^{N} \frac{a_i\, b_i}{\sigma_i^2}$$

$$\left| \underline{\mathbf{a}} - \underline{\mathbf{b}} \right|^2 = \sum_{i=1}^{N} \left(\frac{a_i - b_i}{\sigma_i} \right)^2 .$$

- So the (distance)^2 between data $\underline{\mathbf{x}}$ and parameterised model $\underline{\boldsymbol{\mu}}(\alpha)$ is:

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{X_i - \mu_i(\alpha)}{\sigma_i} \right)^2 = \left| \underline{\mathbf{x}} - \underline{\mu}(\alpha) \right|^2 .$$



Scaling a Pattern to fit the Data

- Minimise χ^2 -> pick model closest to the data.
- Scaling a pattern: $\underline{\mu}(\alpha) = \alpha\,\underline{\mathbf{p}}$:

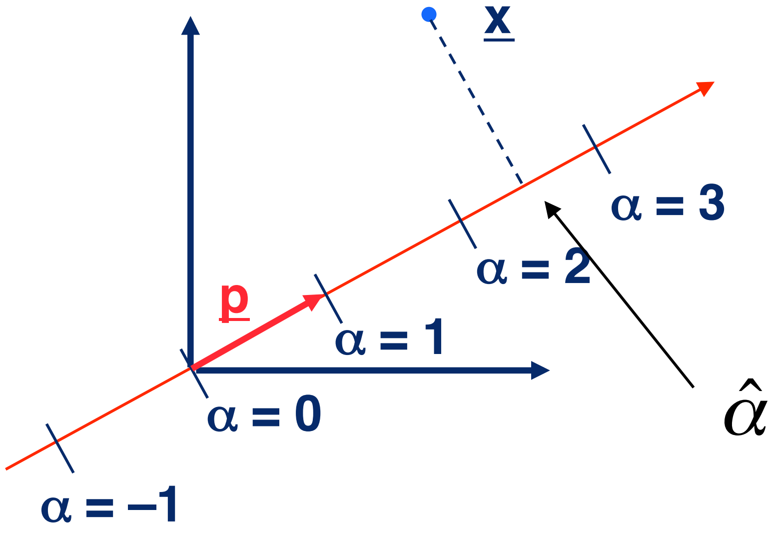
$$\langle x_i \rangle = \mu_i(\alpha) = \alpha\, p_i$$

- The pattern $\underline{\mathbf{p}}$ is a **vector** in data space.
- The model is a **line** in data space, multiples of **p**.
- The best fit is the point along the line closest to the data $\underline{\mathbf{x}}$

$$\hat{\alpha} = \frac{\sum x_i\, P_i / \sigma_i^2}{\sum P_i^2 / \sigma_i^2} = \frac{\underline{\mathbf{x}} \bullet \underline{\mathbf{p}}}{\underline{\mathbf{p}} \bullet \underline{\mathbf{p}}}$$

$$\underline{\mu}(\hat{\alpha}) = \hat{\alpha}\, \underline{\mathbf{p}} = \left(\frac{\underline{\mathbf{x}} \bullet \underline{\mathbf{p}}}{\underline{\mathbf{p}} \bullet \underline{\mathbf{p}}} \right) \underline{\mathbf{p}} = \left(\underline{\mathbf{x}} \bullet \underline{\mathbf{e}}_p \right) \underline{\mathbf{e}}_p$$

$$\underline{\mathbf{e}}_p \equiv \frac{\underline{\mathbf{p}}}{\left| \underline{\mathbf{p}} \right|}$$



Stretching the Basis Vectors

Using the vector notation,

$$\hat{\alpha} = \frac{\underline{\mathbf{p}} \bullet \underline{\mathbf{x}}}{\underline{\mathbf{p}} \bullet \underline{\mathbf{p}}} = \frac{\sum_i \sum_j x^i\, p^j\, g_{i\,j}}{\sum_i \sum_j p^i\, p^j\, g_{i\,j}} = \frac{\sum_i x^i\, p^i \big/ \sigma_i^{\,2}}{\sum_i \left(p^i\right)^2 \big/ \sigma_i^{\,2}}$$

$$\underline{\mathbf{e}}_1 = \{1,0,\ldots,0\}$$
$$\underline{\mathbf{e}}_2 = \{0,1,\ldots,0\}$$
$$\ldots$$
$$\underline{\mathbf{e}}_N = \{0,0,\ldots,1\}$$

So the $\underline{\mathbf{e}}_i$ basis vectors are **orthogonal but not unit length**, corresponding to the metric

$$g_{i\,j} = \underline{e}_i \bullet \underline{e}_j = \frac{1}{\sigma_i^2}\delta_{i\,j}$$

i.e. σ_i **is the natural unit of distance** on the i_{th} axis of data space!

We can "stretch" axis i by factor σ_i to define a new set of **ortho-normal basis vectors $\underline{\mathbf{b}}_i$** :

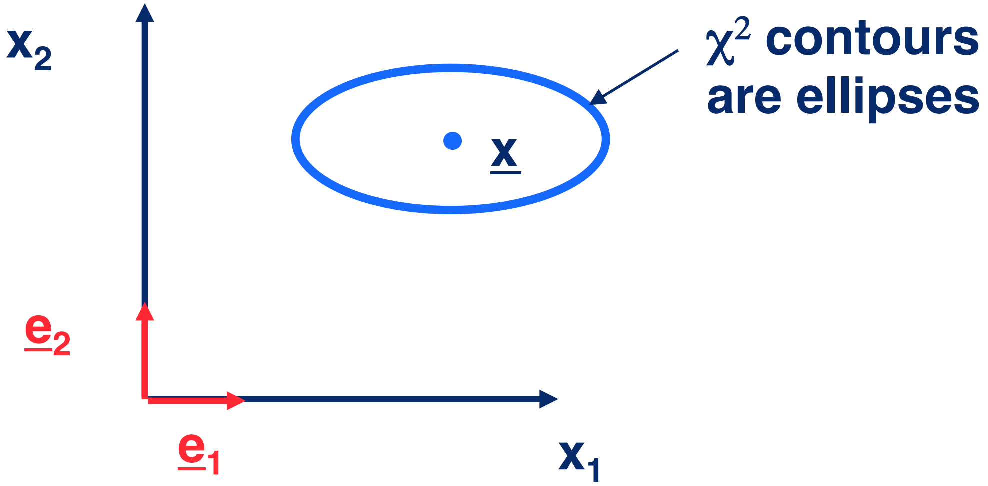
$$\underline{\mathbf{b}}_i \equiv \sigma_i\, \underline{\mathbf{e}}_i \qquad \underline{\mathbf{b}}_i \bullet \underline{\mathbf{b}}_j = \delta_{i\,j}$$

$$\underline{\mathbf{b}}_1 = \{\sigma_1,0,\ldots,0\}$$
$$\underline{\mathbf{b}}_2 = \{0,\sigma_2,\ldots,0\}$$
$$\ldots$$
$$\underline{\mathbf{b}}_N = \{0,0,\ldots,\sigma_N\}$$

Stretch basis vectors to make χ^2 ellipses become circles

Old basis vectors:

$$\underline{\mathbf{x}} = \sum_{i=1}^{N} x_i\, \underline{\mathbf{e}}_i \qquad g_{ij} = \underline{\mathbf{e}}_i \bullet \underline{\mathbf{e}}_j = \frac{\delta_{ij}}{\sigma_i^2}$$

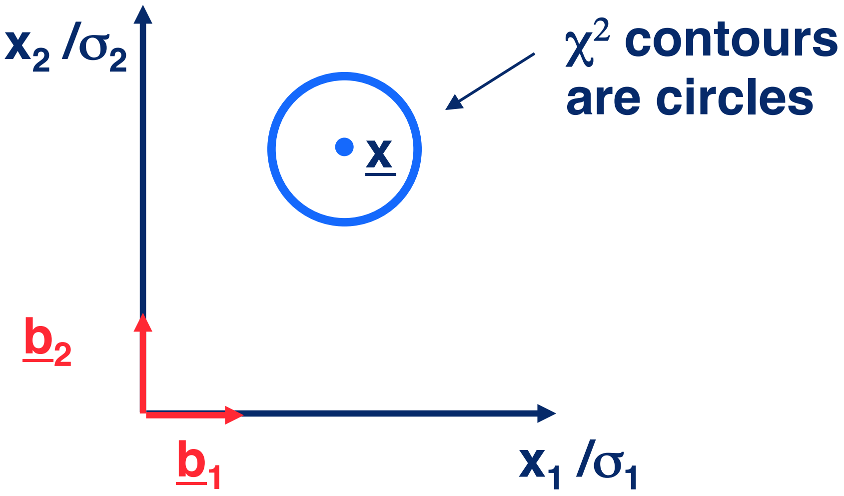


χ^2 contours are ellipses

"Stretched" basis vectors are orthonormal:

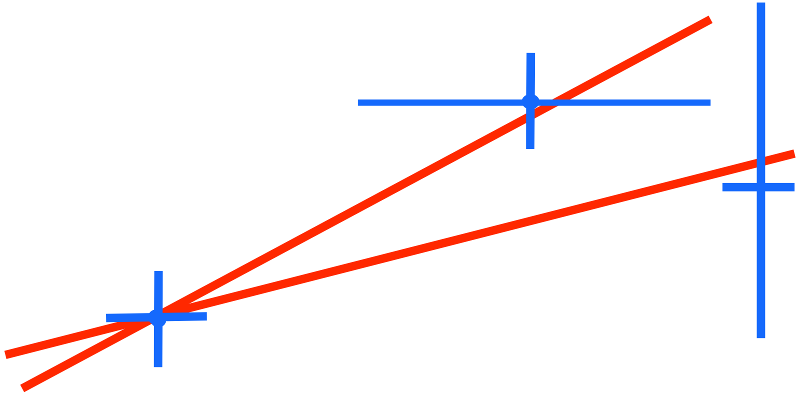
$$\underline{\mathbf{b}}_i \equiv \sigma_i\, \underline{\mathbf{e}}_i \qquad g_{ij} \equiv \underline{\mathbf{b}}_i \bullet \underline{\mathbf{b}}_j = \delta_{ij}$$

$$\underline{\mathbf{x}} = \sum_{i=1}^{N} \left\langle \mathbf{x},\, \underline{\mathbf{b}}_i \right\rangle \underline{\mathbf{b}}_i = \sum_{i=1}^{N} \frac{x_i}{\sigma_i}\, \underline{\mathbf{b}}_i$$



χ^2 contours are circles

Error Bars in both X and Y



Wrong ways to fit a line :

1. $y(x) = a\ x + b \quad (\sigma_x = 0)$

2. $x(y) = c\ y + d \quad (\sigma_y = 0)$

3. split difference between 1 and 2.

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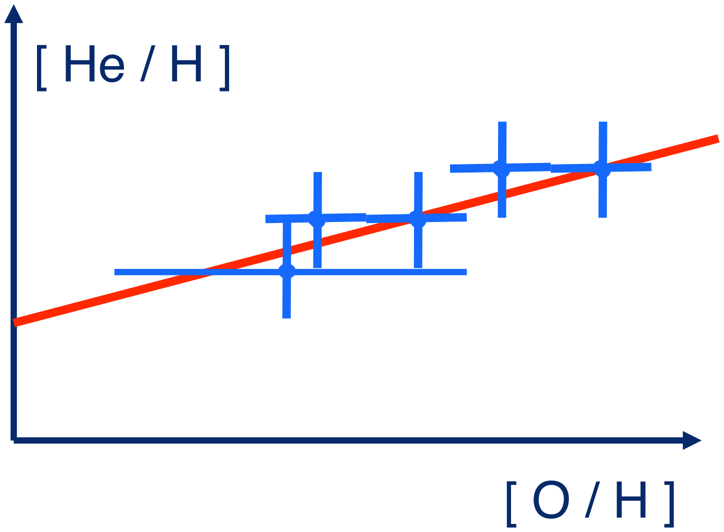
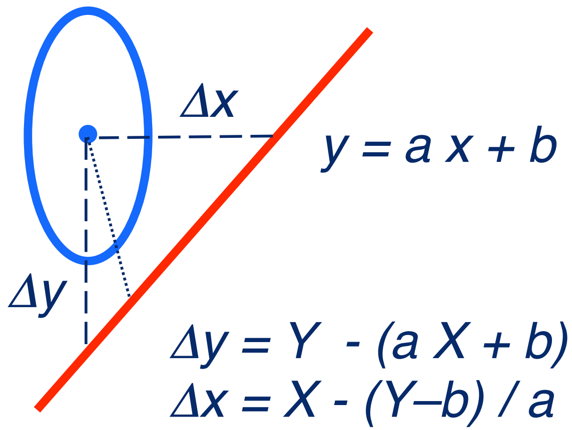
Extrapolate fit line to [O / H] = 0.



Line Fit with error bars in both X and Y

Data: $X \pm \sigma_X \quad Y \pm \sigma_Y$

Model: $y = a\,x + b$



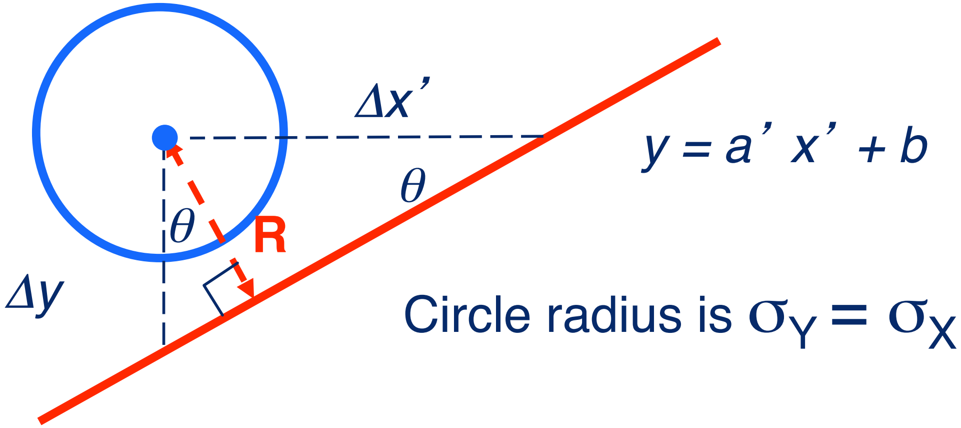
$\Delta y = Y - (a\,X + b)$
$\Delta x = X - (Y - b)\,/\,a$

For $\sigma_X \neq \sigma_Y$, **where is the point of closest approach ?**

Not obvious.

Horizontal stretch by factor σ_Y / σ_X
makes the probability cloud round.

Also changes the slope: a => a'



Circle radius is $\sigma_Y = \sigma_{X'}$

$$\Delta x' = \frac{\sigma_Y}{\sigma_X}\,\Delta x \qquad a' = \frac{\Delta y}{\Delta x'} = \frac{\sigma_X}{\sigma_Y}\,a = \tan\theta$$

Closest approach at $R = \Delta y \cos\theta$

$$\left(\frac{R}{\Delta y}\right)^2 = \frac{\cos^2\theta}{\cos^2\theta + \sin^2\theta} = \frac{1}{1+\tan^2\theta} = \frac{\sigma_Y^2}{\sigma_Y^2 + a^2\sigma_X^2}$$

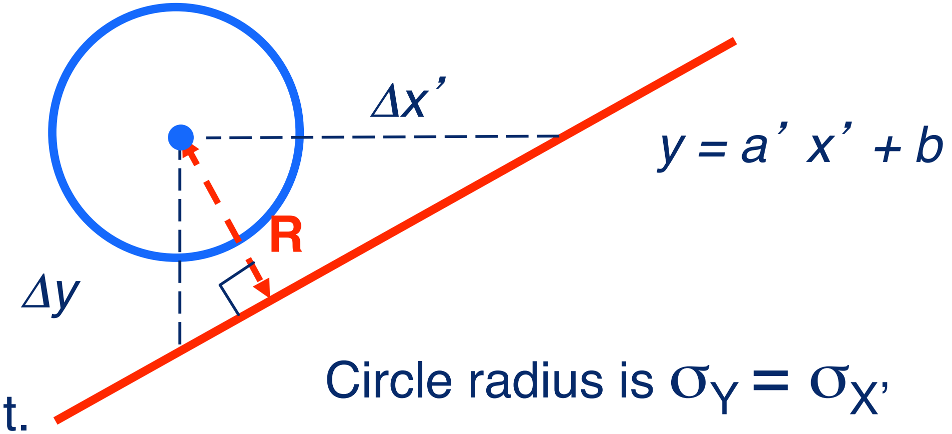
$$\left(\frac{R}{\sigma_Y}\right)^2 = \left(\frac{\Delta y}{\sigma_Y}\,\frac{R}{\Delta y}\right)^2 = \frac{\Delta y^2}{\sigma_Y^2 + a^2\sigma_X^2}$$

Defining χ^2 for errors in both X and Y

Horizontal stretch makes probability cloud round.

Distance *R* at closest approach is :

$$\left(\frac{R}{\sigma_Y}\right)^2 = \frac{\Delta y^2}{\sigma_Y^2 + a^2\sigma_X^2}$$



Circle radius is $\sigma_Y = \sigma_{X'}$

Note: Need a different stretch for each data point.

Total (distance)^2 in the *2 N* - dimensional data space:

$$\chi^2 = \sum_{i=1}^{N}\left[\left(\frac{\varepsilon(Y_i)}{\sigma(Y_i)}\right)^2 + \left(\frac{\varepsilon(X_i')}{\sigma(X_i')}\right)^2\right] = \sum_{i-1}^{N}\left(\frac{\varepsilon(Y_i)^2 + \varepsilon(X_i')^2}{\sigma^2(Y_i)}\right)$$

$$= \sum_{i=1}^{N}\left(\frac{R}{\sigma(Y_i)}\right)^2 = \sum_{i=1}^{N}\frac{\left(Y_i - (a\,X_i + b)\right)^2}{\sigma^2(Y_i) + a^2\sigma^2(X_i)}$$