# Linear Regression With Errors in Both Variables 

T. Ihn

21. November 2016

Background information and model: We measure data points $\left(x_{\mathrm{m} i}, y_{\mathrm{m} i}\right)$, where both quantities are independently measured. For example, $x_{\mathrm{m} i}$ could be the measured value of a magnetic field and $y_{\mathrm{m} i}$ would be the the corresponding Hall voltage. The special situation considered here is that both quantities have an additive error, i.e.

$$
\begin{aligned}
x_{\mathrm{m} i} & =x_{i}+\epsilon_{i} \\
y_{\mathrm{m} i} & =y_{i}+\eta_{i}
\end{aligned}
$$

The errors $\epsilon_{i}$ and $\eta_{i}$ are assumed to be statistically independent.
We consider the case where a linear functional relationship exists between the exact values $y_{i}$ and $x_{i}$. Therefore,

$$
\begin{equation*}
y_{i}=\alpha x_{i}+\beta \tag{1}
\end{equation*}
$$

is considered to be a valid model for the measured data with parameters $\alpha$ and $\beta$ independent of the measured data point. The probability distributions for $\epsilon_{i}$ and $\eta_{i}$ are given by normal distributions

$$
\begin{aligned}
\operatorname{pdf}\left(\epsilon_{i} \mid \sigma_{x}\right) d \epsilon_{i} & =\mathcal{N}\left(\epsilon_{i} ; 0, \sigma_{x}\right) d \epsilon_{i} \\
\operatorname{pdf}\left(\eta_{i} \mid \sigma_{y}\right) d \eta_{i} & =\mathcal{N}\left(\eta_{i} ; 0, \sigma_{y}\right) d \eta_{i} .
\end{aligned}
$$

The error bars $\sigma_{x}$ and $\sigma_{y}$ are assumed to be known, and to be the same for all data points. An example dataset is shown in Fig. 1.

General difficulty of this problem. We compare this problem to the standard linear regression case with the $N$ measured data points ( $x_{\mathrm{m} i}, y_{\mathrm{m} i}$ ), where all the $x_{\mathrm{m} i} \equiv x_{i}$ are known exactly. In this case there remain $N$ unknown exact values $y_{i}$. Given the linear relation (1), knowledge of the two unknown parameters $\alpha$ and $\beta$ would allow us to immediately determine all the unknown exact $y_{i}$ values from the $\left\{x_{i}\right\}$. The linear fitting function therefore reduces the $N$ unknown values $\left\{y_{i}\right\}$ to only two unknown parameters. We can extract estimates and uncertainties for these two paramters $\alpha$ and $\beta$ from $N>2$ data points.

Now we see the general difficulty of having errors in both variables. Having $N$ measured data points $\left(x_{\mathrm{m} i}, y_{\mathrm{m} i}\right)$ we start with $2 N$ unknowns, i.e., the $N$ pairs of exact values $\left\{\left(x_{i}, y_{i}\right)\right\}$.


Abbildung 1: Data with errors in both variables. The goal is to find a straight line fit taking the errors in both variables into account. For this data, $\sigma_{x}=0.5$ and $\sigma_{y}=0.8$ are known.

Using the linear relation between the $x_{i}$ and the $y_{i}$ gives $N$ equations, but two additional parameters, leading to a net reduction of the number of unknown parameters to $N+2$, e.g. the $N$ values $\left\{x_{i}\right\}$ and the two paramters $\alpha$ and $\beta$. However, we still have only $N$ data points, i.e., the system is still underdetermined (rather than overdetermined). This means that we cannot get a reasonable linear fit and extract the parameters $\alpha$ and $\beta$ without supplying additional information about some of the $N+2$ unknown parameters. It is clear that a similar problem would arise, if the errors $\sigma_{x}$ and $\sigma_{y}$ were unknown as well. This would further increase the number of unknown parameters to $N+4$.

A different view of the same problem. We now follow Gull ${ }^{1}$ in looking at the same problem from a different angle, which highlights the symmetry between the $x$ - and $y$-values.

[^0]Suppose we consider dimensionless quantities

$$
\begin{aligned}
x_{i}^{\prime} & =\frac{x_{i}-x_{0}}{r_{x}} \\
y_{i}^{\prime} & =\frac{y_{i}-y_{0}}{r_{y}}
\end{aligned}
$$

where $x_{0}$ and $y_{0}$ are location parameters and $r_{x}>0$ and $r_{y}>0$ are scale parameters. The functional relationship (1) between $x_{i}^{\prime}$ and $y_{i}^{\prime}$ can then be written as

$$
r_{y} y_{i}^{\prime}+y_{0}=\alpha\left(r_{x} x_{i}^{\prime}+x_{0}\right)+\beta
$$

Identifying

$$
\alpha= \pm \frac{r_{y}}{r_{x}} \quad \text { and } \quad \beta=y_{0}-\alpha x_{0}
$$

we find the line with slope one (or minus one)

$$
y_{i}^{\prime}= \pm x_{i}^{\prime}
$$

We may therefore say, instead of looking for a slope parameter $\alpha$ and an intersection parameter $\beta$, we look for location parameters $x_{0}, y_{0}$ and scale parameters $r_{x}, r_{y}$ that would transform our data to a line of slope one (or -1 , if $\alpha<0$ ) extending in $x_{i}^{\prime}$ and $y_{i}^{\prime}$ symmetrically around the origin. The error variables $\epsilon_{i}$ and $\eta_{i}$ transform according to

$$
\epsilon_{i}^{\prime}=\frac{\epsilon_{i}}{r_{x}} \quad \text { and } \quad \eta_{i}^{\prime}=\frac{\eta_{i}}{r_{y}}
$$

Correspondingly, their distribution functions are

$$
\operatorname{pdf}\left(\epsilon_{i}^{\prime}\right)=\mathcal{N}\left(\epsilon_{i}^{\prime} ; 0, \sigma_{x}^{\prime}\right) \quad \text { and } \quad \operatorname{pdf}\left(\eta_{i}^{\prime}\right)=\mathcal{N}\left(\eta_{i}^{\prime} ; 0, \sigma_{y}^{\prime}\right)
$$

with

$$
\sigma_{x}^{\prime}=\frac{\sigma_{x}}{r_{x}} \quad \text { and } \quad \sigma_{y}^{\prime}=\frac{\sigma_{y}}{r_{y}}
$$

and the measured data are

$$
\frac{x_{\mathrm{m} i}-x_{0}}{r_{x}}=x_{i}^{\prime}+\epsilon_{i}^{\prime} \quad \text { and } \quad \frac{y_{\mathrm{m} i}-y_{0}}{r_{y}}=y_{i}^{\prime}+\eta_{i}^{\prime}
$$

The likelihood function. We further assume the two uncertainties $\eta_{i}^{\prime}$ and $\epsilon_{i}^{\prime}$ to be statistically independent and obtain the joint distribution

$$
\operatorname{pdf}\left(\epsilon_{i}^{\prime}, \eta_{i}^{\prime} \mid \sigma_{x}^{\prime}, \sigma_{y}^{\prime}\right) d \epsilon_{i}^{\prime} d \eta_{i}^{\prime}=\mathcal{N}\left(\epsilon_{i}^{\prime} ; 0, \sigma_{x}^{\prime}\right) \mathcal{N}\left(\eta_{i}^{\prime} ; 0, \sigma_{y}^{\prime}\right) d \epsilon_{i}^{\prime} d \eta_{i}^{\prime}
$$

As a result we have the samping distribution for $N$ data points

$$
\begin{aligned}
& \operatorname{pdf}\left(\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\} \mid\left\{x_{i}\right\}, x_{0}, y_{0}, r_{x}, r_{y}, \sigma_{x}^{\prime}, \sigma_{y}^{\prime}\right) d^{N} x_{\mathrm{m}} d^{N} y_{\mathrm{m}} \\
& \quad=\frac{d^{N} x_{\mathrm{m} i} d^{N} y_{\mathrm{m} i}}{\left(r_{x} r_{y}\right)^{N}} \prod_{i=1}^{N} \mathcal{N}\left(\frac{x_{\mathrm{m} i}-x_{0}}{r_{x}} ; x_{i}^{\prime}, \sigma_{x}^{\prime}\right) \mathcal{N}\left(\frac{y_{\mathrm{m} i}-y_{0}}{r_{y}} ; x_{i}^{\prime}, \sigma_{y}^{\prime}\right) \\
& = \\
& \frac{d^{N} x_{\mathrm{m}} d^{N} y_{\mathrm{m} i}}{\left(2 \pi \sigma_{x}^{\prime} \sigma_{y}^{\prime} r_{x} r_{y}\right)^{N}} \exp \left[-\frac{1}{2}\left(\frac{\sum_{i=1}^{N}\left(x_{\mathrm{m} i}-x_{i}\right)^{2}}{\sigma_{x}{ }^{2}}+\frac{\left.\sum_{i=1}^{N}\left(y_{\mathrm{m} i}-y_{0}-r_{y}\left(x_{i}-x_{0}\right) / r_{x}\right)^{2}\right\rangle}{\sigma_{y}{ }^{2}}\right)\right] .
\end{aligned}
$$

This likelihood function contains the $N$ parameters $x_{i}$ as so-called nuisance parameters. ${ }^{2}$ In addition, we have replaced the original two parameters $\alpha$ and $\beta$ by four new parameters $x_{0}$, $y_{0}, r_{x}$, and $r_{y}$, which may seem a bit awkward at a first glance. However, we will see below that this allows a formulation of the problem that is symmetric under the exchange of $x$ and $y$, a symmetry that naturally appears in the problem, because it is usually arbitrary, which of the two measured quantities we call $x$ and which $y$.

Prior distributions for $x_{0}, y_{0}, r_{x}$, and $r_{y}$. In order to make further progress, we need a prior distribution function for the $N+4$ parameters

$$
\operatorname{pdf}\left(\left\{x_{i}\right\}, x_{0}, y_{0}, r_{x}, r_{y}\right)=\operatorname{pdf}\left(x_{0}, y_{0}, r_{x}, r_{y}\right) \operatorname{pdf}\left(\left\{x_{i}\right\} \mid x_{0}, y_{0}, r_{x}, r_{y}\right)
$$

We choose

$$
\operatorname{pdf}\left(x_{0}, y_{0}, \ln r_{x}, \ln r_{y}\right) \propto d x_{0} d y_{0} d\left(\ln r_{x}\right) d\left(\ln r_{y}\right)
$$

which is a completely uninformative prior for the location parameters $x_{0}$ and $y_{0}$, and for the scale parameters $r_{x}>0$ and $r_{y}>0$. For the latter, a uniform distribution in the logarithm ensures that these quantities are positive. Such a prior is called Jeffreys prior. ${ }^{3}$

Prior distribution for the $\left\{x_{i}\right\}$. There remains a prior to be found for the unknown $\left\{x_{i}\right\}$. Using a completely uninformative (constant) prior for these variables would leave us with an unsolvable underdetermined problem, as discussed above. We therefore have to provide additional information here about the $\left\{x_{i}\right\}$. We will therefore assume that all the $x_{i}$ are with large probability within the range $\pm r_{x}$ around $x_{0}$. We see that this leaves great freedom for the $x_{i}$ to vary within the range, where their values are expected. This is the additional information that we supply to return to an overdetermined problem in the end.

In order to implement this thought, we use the product of gaussians

$$
\operatorname{pdf}\left(\left\{x_{i}\right\} \mid x_{0}, y_{0}, r_{x}, r_{y}\right)=\prod_{i=1}^{N} \mathcal{N}\left(x_{i} ; x_{0}, r_{x}\right)=\frac{1}{\left(2 \pi r_{x}^{2}\right)^{N / 2}} \exp \left[-\frac{1}{2} \frac{\sum_{i=1}^{N}\left(x_{i}-x_{0}\right)^{2}}{r_{x}^{2}}\right]
$$

[^1]Note that this prior is completely symmetric in $x$ and $y$, since our choice of parameters ensures that $\left(x_{i}-x_{0}\right) / r_{x}=\left(y_{i}-y_{0}\right) / r_{y}$. It therefore conforms with our aim of a formulation of the problem symmetric under the exchange of $x$ and $y$.

It is a general property of models with nuisance parameters, that a prior distribution needs to be specified, which will influence the final result. This prior allows us to marginalize the nuisance parameters later on. The choice of a gaussian prior in our specific case is less a matter of necessity, but of convenience. We will see that it later allows an analytic marginalization of the nuisance parameters.

Joint distribution. We can now write down the joint distribution function for data and parameters as

$$
\begin{aligned}
& \operatorname{pdf}\left(\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\},\left\{x_{i}\right\}, x_{0}, y_{0}, \ln r_{x}, \ln r_{y} \mid \sigma_{x}, \sigma_{y}\right) \\
& =\frac{1}{\left(8 \pi^{3} \sigma_{x}^{2} \sigma_{y}^{2} r_{x}^{2}\right)^{N / 2}} \\
& \quad \times \exp \left[-\frac{1}{2} \sum_{i=1}^{N}\left(\frac{\left(x_{\mathrm{m} i}-x_{i}\right)^{2}}{\sigma_{x}^{2}}+\frac{\left(y_{\mathrm{m} i}-y_{0}-r_{y}\left(x_{i}-x_{0}\right) / r_{x}\right)^{2}}{\sigma_{y}^{2}}+\frac{\left(x_{i}-x_{0}\right)^{2}}{r_{x}^{2}}\right)\right] .
\end{aligned}
$$

Integrating out (marginalizing) the nuisance parameters $x_{i}$. In the next step we integrate out the nuisance parameters $x_{i}$. This multidimensional integral separates into $N$ integrals of the form

$$
\begin{aligned}
& r_{x} \int d x_{i}^{\prime} \exp \left[-\frac{1}{2}\left(\frac{\left(x_{\mathrm{m} i}^{\prime}-x_{i}^{\prime}\right)^{2}}{{\sigma_{x}^{\prime}}^{2}}+\frac{\left(y_{\mathrm{m} i}^{\prime}-x_{i}^{\prime}\right)^{2}}{\sigma_{y}^{\prime 2}}+{x_{i}^{\prime}}^{2}\right)\right] \\
& \quad=\frac{\sqrt{2 \pi} \sigma_{x}^{\prime} \sigma_{y}^{\prime} r_{x}}{\sqrt{{\sigma_{x}^{\prime}}^{2}+{\sigma_{y}^{\prime}}^{2}+{\sigma_{x}^{\prime}}^{2}{\sigma_{y}^{\prime}}^{2}}} \times \exp \left[-\frac{\left(1+{\sigma_{y}^{\prime}}^{2}\right) x_{\mathrm{m} i}^{\prime}{ }^{2}-2 x_{\mathrm{m} i}^{\prime} y_{\mathrm{m} i}^{\prime}+\left(1+{\sigma_{x}^{\prime}}^{2}\right) y_{\mathrm{m} i}^{\prime}}{\left.2{\left(\sigma_{x}^{\prime}\right.}^{2}+{\sigma_{y}^{\prime}}^{2}+{\sigma_{x}^{\prime}}^{2}{\sigma_{y}^{\prime}}^{2}\right)}\right],
\end{aligned}
$$

where the exponent is a quadratic form of $x_{0}$ and $y_{0}$. The result of the $N$-fold integration is therefore the joint distribution for the data and the 4 remaining parameters

$$
\begin{aligned}
& \operatorname{pdf}\left(\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, x_{0}, y_{0}, \ln r_{x}, \ln r_{y} \mid \sigma_{x}, \sigma_{y}\right) \\
&=\left(\frac{1}{4 \pi^{2}\left(r_{y}^{2} \sigma_{x}^{2}+r_{x}^{2} \sigma_{y}^{2}+\sigma_{x}^{2} \sigma_{y}^{2}\right)}\right)^{N / 2} \\
& \times \exp \left[-\frac{\sum_{i=1}^{N}\left[\left(r_{y}^{2}+\sigma_{y}^{2}\right)\left(x_{\mathrm{m} i}-x_{0}\right)^{2}-2 r_{x} r_{y}\left(x_{\mathrm{m} i}-x_{0}\right)\left(y_{\mathrm{m} i}-y_{0}\right)+\left(r_{x}^{2}+\sigma_{x}^{2}\right)\left(y_{\mathrm{m} i}-y_{0}\right)^{2}\right]}{2\left(r_{y}^{2} \sigma_{x}^{2}+r_{x}^{2} \sigma_{y}^{2}+\sigma_{x}^{2} \sigma_{y}^{2}\right)}\right],
\end{aligned}
$$

which is a bivariate gaussian distribution for $x_{0}$ and $y_{0}$. Note also the symmetry of the joint distribution with respect of an exchange of $x$ and $y$.

Sufficient statistics. The sum in the numerator of the exponent can be transformed into sample averages giving

$$
\begin{aligned}
& \operatorname{pdf}\left(\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, x_{0}, y_{0}, \ln r_{x}, \ln r_{y} \mid \sigma_{x}, \sigma_{y}\right) \\
& \quad=\left(\frac{1}{4 \pi^{2}\left(r_{y}^{2} \sigma_{x}^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}\right)}\right)^{N / 2} \\
& \times \exp \left[-\frac{N}{2} \frac{\left(r_{y}^{2}+\sigma_{y}{ }^{2}\right)\left(x_{0}-\overline{x_{\mathrm{m} i}}\right)^{2}-2 r_{x} r_{y}\left(x_{0}-\overline{x_{\mathrm{m} i}}\right)\left(y_{0}-\overline{y_{\mathrm{m}}}\right)+\left(r_{x}^{2}+\sigma_{x}{ }^{2}\right)\left(y_{0}-\overline{y_{\mathrm{m}} i}\right)^{2}}{r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}}\right] \\
& \times \exp \left[-\frac{N}{2} \frac{\left(r_{y}^{2}+\sigma_{y}{ }^{2}\right) \operatorname{Var}\left(x_{\mathrm{m} i}\right)-2 r_{x} r_{y} \sqrt{\operatorname{Var}\left(x_{\mathrm{m} i}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)} \rho+\left(r_{x}^{2}+\sigma_{x}{ }^{2}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)}{r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}}\right] .
\end{aligned}
$$

We see that the quantities $\overline{x_{\mathrm{m} i}}, \overline{y_{\mathrm{m} i}}, \operatorname{Var}\left(x_{\mathrm{m} i}\right), \operatorname{Var}\left(y_{\mathrm{m} i}\right)$, and $\rho$ are a sufficient statistic for the problem, like in standard linear regression where errors are only in $y$.

We note here that the exponent of the first exponential factor can be expressed as

$$
-\frac{N}{2}\binom{x_{0}-\overline{x_{\mathrm{m} i}}}{y_{0}-\overline{y_{\mathrm{m} i}}} \underbrace{\overline{r_{y}^{2} \sigma_{x}^{2}+r_{x}^{2} \sigma_{y}^{2}+\sigma_{x}^{2} \sigma_{y}^{2}}\left(\begin{array}{cc}
r_{y}^{2}+\sigma_{y}^{2} & -r_{x} r_{y} \\
-r_{x} r_{y} & r_{x}^{2}+\sigma_{x}^{2}
\end{array}\right)}_{:=M}\binom{x_{0}-\overline{x_{\mathrm{m} i}}}{y_{0}-\overline{y_{\mathrm{m} i}}},
$$

where $\operatorname{det}(M)=1$.
Posterior distribution and estimates of the shift parameters. The posterior distribution for $x_{0}, y_{0}, r_{x}, r_{y}$ given the data is then

$$
\begin{aligned}
& \operatorname{pdf}\left(x_{0}, y_{0}, \ln r_{x}, \ln r_{y} \mid\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, \sigma_{x}, \sigma_{y}\right) \\
& \propto\left(r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}\right)^{-N / 2} \\
& \times \exp \left[-\frac{N}{2} \frac{\left(r_{y}^{2}+\sigma_{y}{ }^{2}\right)\left(x_{0}-\overline{x_{\mathrm{m} i}}\right)^{2}-2 r_{x} r_{y}\left(x_{0}-\overline{x_{\mathrm{m} i}}\right)\left(y_{0}-\overline{y_{\mathrm{m} i}}\right)+\left(r_{x}^{2}+\sigma_{x}{ }^{2}\right)\left(y_{0}-\overline{y_{\mathrm{m} i}}\right)^{2}}{r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}}\right] \\
& \times \exp \left[-\frac{N}{2} \frac{\left(r_{y}^{2}+\sigma_{y}{ }^{2}\right) \operatorname{Var}\left(x_{\mathrm{m} i}\right)-2 r_{x} r_{y} \sqrt{\operatorname{Var}\left(x_{\mathrm{m} i}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)} \rho+\left(r_{x}^{2}+\sigma_{x}{ }^{2}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)}{r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}}\right] .
\end{aligned}
$$

From this posterior we find the estimates for $x_{0}$ and $y_{0}$ with their uncertainties

$$
\begin{array}{ccc}
\hat{x}_{0}=\left\langle x_{0}\right\rangle=\overline{x_{\mathrm{m} i}} & \text { and } & \hat{y}_{0}=\left\langle y_{0}\right\rangle=\overline{y_{\mathrm{m} i}} \\
\left\langle\Delta x_{0}^{2}\right\rangle=\frac{\sigma_{x}^{2}+r_{x}^{2}}{N} & \text { and } & \left\langle\Delta y_{0}^{2}\right\rangle=\frac{\sigma_{y}^{2}+r_{y}^{2}}{N} \\
& \left\langle\Delta x_{0} \Delta y_{0}\right\rangle=\frac{r_{x} r_{y}}{N} &
\end{array}
$$

Note that the estimates taken to be the mean values of $x_{0}$ and $y_{0}$ calculated with the posterior distribution are at the same time maximizing the posterior distribution for any values of $r_{x}$ and $r_{y}$. These estimates allow us to plot the shifted data as shown in Fig. 2.


Abbildung 2: Data shifted by $x_{0}=\overline{x_{\mathrm{m} i}}=10.68$ and $y_{0}=\overline{y_{\mathrm{m} i}}=25.95$.
Estimating the scaling parameters. Integrating out $x_{0}$ and $y_{0}$ from the posterior distribution gives

$$
\begin{aligned}
& \operatorname{pdf}\left(\ln r_{x}, \ln r_{y} \mid\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, \sigma_{x}, \sigma_{y}\right) \\
& \quad \propto\left(r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}\right)^{-N / 2} \\
& \quad \times \exp \left[-\frac{N}{2} \frac{\left(r_{y}^{2}+\sigma_{y}{ }^{2}\right) \operatorname{Var}\left(x_{\mathrm{m} i}\right)-2 r_{x} r_{y} \sqrt{\operatorname{Var}\left(x_{\mathrm{m} i}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)} \rho+\left(r_{x}^{2}+\sigma_{x}{ }^{2}\right) \operatorname{Var}\left(y_{\mathrm{m} i}\right)}{r_{y}^{2} \sigma_{x}{ }^{2}+r_{x}^{2} \sigma_{y}{ }^{2}+\sigma_{x}{ }^{2} \sigma_{y}{ }^{2}}\right] .
\end{aligned}
$$

We see here that $\operatorname{Var}\left(x_{\mathrm{m} i}\right)$ and $\operatorname{Var}\left(y_{\mathrm{m} i}\right)$ appear as natural scales of the problem. If we introduce

$$
r_{x}^{\prime}=\frac{r_{x}}{\sqrt{\operatorname{Var}\left(x_{\mathrm{m} i}\right)}}, \quad r_{y}^{\prime}=\frac{r_{y}}{\sqrt{\operatorname{Var}\left(y_{\mathrm{m} i}\right)}}, \quad \sigma_{x}^{\prime}=\frac{\sigma_{x}}{\sqrt{\operatorname{Var}\left(x_{\mathrm{m} i}\right)}}, \quad \sigma_{y}^{\prime}=\frac{\sigma_{y}}{\sqrt{\operatorname{Var}\left(y_{\mathrm{m} i}\right)}},
$$

we obtain

$$
\begin{aligned}
& \operatorname{pdf}\left(\ln r_{x}^{\prime}, \ln r_{y}^{\prime} \mid\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, \sigma_{x}^{\prime}, \sigma_{y}^{\prime}\right) \\
& \propto\left(r_{y}^{\prime 2}{\sigma_{x}^{\prime 2}}^{2}+{r_{x}^{\prime}}^{2}{\sigma_{y}^{\prime 2}}^{2}+{\sigma_{x}^{\prime}}^{2} \sigma_{y}^{\prime 2}\right)^{-N / 2} \\
& \times \exp \left[-\frac{N}{2} \frac{\left({r_{y}^{\prime}}^{2}+\sigma_{y}^{\prime 2}\right)-2 r_{x}^{\prime} r_{y}^{\prime} \rho+\left({r_{x}^{\prime}}^{2}+{\sigma_{x}^{\prime}}^{2}\right)}{r_{y}^{\prime 2} \sigma_{x}^{\prime 2}+r_{x}^{\prime 2} \sigma_{y}^{\prime 2}+{\sigma_{x}^{\prime 2}}^{2} \sigma_{y}^{\prime 2}}\right] .
\end{aligned}
$$

We may now estimate the parameters $r_{x}^{\prime}$ and $r_{y}^{\prime}$ from the negative logarithm of this posterior function numerically. The example for our data is shown in Fig. 3. We may check our result


Abbildung 3: Logarithm of the posterior distribution for $r_{x}$ and $r_{y}$. The minimum of this function is at $r_{x}^{\prime}=r_{y}^{\prime}=0.95$. The red contour line at the value 1 may be used for estimating the standard errors in these quantities.
by calculating the corresponding estimates for $r_{x}$ and $r_{y}$. The data can then be plotted in the scaled coordinates as shown in Fig. 4.

Estimating the slope $\alpha$ of the data. Changing variables to $\alpha^{\prime}=r_{y}^{\prime} / r_{x}^{\prime}$ and $R^{\prime}=\sqrt{r_{x}^{\prime} r_{y}^{\prime}}$ gives

$$
r_{x}^{\prime}=\frac{R^{\prime}}{\sqrt{\alpha^{\prime}}} \quad \text { and } \quad r_{y}^{\prime}=R^{\prime} \sqrt{\alpha^{\prime}}
$$



Abbildung 4: The original data shifted by ( $x_{0}, y_{0}$ ) and scaled by the estimated $r_{x}$ and $r_{y}$. The red line corresponds to the diagonal along which the data are expected to be scattered.

It leads to

$$
\begin{aligned}
& \operatorname{pdf}\left(\ln \alpha^{\prime}, \ln R^{\prime} \mid\left\{x_{\mathrm{m} i}, y_{\mathrm{m} i}\right\}, \sigma_{x}^{\prime}, \sigma_{y}^{\prime}\right) \\
& \propto\left(R^{\prime 2} \alpha^{\prime} \sigma_{x}^{\prime 2}+R^{\prime 2} \sigma_{y}^{\prime 2} / \alpha^{\prime}+\sigma_{x}^{\prime 2} \sigma_{y}^{\prime 2}\right)^{-N / 2} \\
& \times \exp \left[-\frac{N}{2} \frac{{R^{\prime}}^{2} \alpha^{\prime 2}-2{R^{\prime}}^{2} \rho \alpha^{\prime}+\left({\sigma_{x}^{\prime}}^{2}+{\sigma_{y}^{\prime}}^{2}\right) \alpha^{\prime}+R^{\prime 2}}{R^{2}{\alpha^{\prime 2}}^{\prime 2}{ }_{x}^{2}+\left({\sigma_{x}^{\prime}}^{\prime}{\sigma_{y}^{\prime 2}}^{2}\right) \alpha^{\prime}+{R^{\prime 2}}^{\prime 2}{ }_{y}^{2}}\right] .
\end{aligned}
$$

The minimum of the negative logarithm of this function shown in Fig. 5 is a direct way to estimate $\alpha^{\prime}$ and its uncertainty.

Estimating the intercept parameter $\beta$. The quantity $\beta$ may now be estimated via the relation $\beta=y_{0}-\alpha x_{0}$ to be

$$
\beta=\overline{y_{\mathrm{m} i}}-\alpha \overline{x_{\mathrm{m} i}} .
$$



Abbildung 5: Negative logarithm of the posterior distribution for $\alpha^{\prime}$ and $R^{\prime}$. The minimum in this figure is found at $\alpha^{\prime}=0.996$ and $R^{\prime}=0.971$. Together with the data variance $\operatorname{Var}\left(x_{\mathrm{m} i}\right)=30.57$ and $\operatorname{Var}\left(y_{\mathrm{m} i}\right)=127.00$ this gives an estimate of the slope $\alpha=2.03$. The red contour line may be used to estimate the errors in the two quantities graphically. We find from the two vertical dashed lines $\alpha^{\prime}=0.996 \pm 0.075$ translating into $\alpha=2.03 \pm 0.15$.

In principle, the uncertainty of the $b$-estimate would need to be calculated from the posterior distribution for $x_{0}, y_{0}$ and $\alpha$. The integration over $x_{0}$ and $y_{0}$ can be performed analytically and gives

$$
\left\langle\Delta \beta^{2}\right\rangle_{x_{0}, y_{0}}=\frac{\sigma_{y}^{2}+\alpha^{2} \sigma_{x}^{2}}{N}
$$

As a shortcut we may use, instead of the numerical integration, using Gauss' error propagation law

$$
\left\langle\Delta \beta^{2}\right\rangle=\frac{\sigma_{y}^{2}+\alpha_{\mathrm{est}}^{2} \sigma_{x}^{2}}{N}+{\overline{x_{\mathrm{m} i}}}^{2}\left\langle\Delta \alpha^{2}\right\rangle
$$

The final result of the fit. Eventually we show the final result of the original data, together with the fitted line determined above in Fig. 6.


Abbildung 6: Final result of the fit to data with errors in $x$ and $y$. The solid red line represents the fit with $\alpha=2.03$ and $\beta=4.3$. The error in $\beta$ is $\Delta \beta=1.6$. The red dashed lines have slopes $\alpha \pm \Delta \alpha=2.03 \pm 0.15$ and $\beta=4.3$. The blue dashed line represents the 'true' curve $y=2 x+5$ from which the data have been generated.

Python code realizing the minimization.

```
from csv import reader
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
from scipy.optimize import fmin
```

```
#
# read data from a csv-file
#
readerout = reader(open("errorxydata.csv","rb"),delimiter=',');
x = list(readerout);
data = np.array(x).astype('float')
xi = data[:,0]
yi = data[:,1]
# Error bars
sigmax = 0.5
sigmay = 0.8
#
# Statistics of the data
#
# number of data points
nn = len(data)
print('\nStatistics of the data:\nN = %1u data points'% (nn))
# mean of x-values
Meanx = np.mean(xi)
print('<x> = %1.2f,% (Meanx))
# mean of y-values
Meany = np.mean(yi)
print('<y> = %1.2f'% (Meany))
# Variance of x-values
Varx = np.var(xi)
print('Var(x) = %1.2f'% (Varx))
# Variance of y-values
Vary = np.var(yi)
print('Var(y) = %1.2f %% (Vary))
# Empirical correlation coefficient
rho = np.corrcoef(xi.T,yi.T)[0,1]
print('rho = %1.4f\n'% (rho))
```

```
# Define the -log-posterior for a and R
def posteriorpdf(parms,sx,sy,rho,n):
    a = parms[0]
    R = parms[1]
    num = R*R*a*a - 2*R*R*rho*a + (sx*sx+sy*sy)*a + R*R
    denom = sx*sx*R*R*a*a + sx*sx*sy*sy*a + R*R*sy*sy
    p = num/denom
    q = sx*sx*R*R*a+sy*sy*R*R/a+sx*sx*sy*sy
    return np.log(R*a) + (n/2.)*np.log(q) + (n/2.)*p
# Minimization of the -log-posterior
print('Estimating scaled parameters:')
parms,Qmin,_,_,_ = fmin(posteriorpdf,[1.,1.],args=(sigmax/np.sqrt(Varx),sigmay/np.sqrt(Vary
aa = parms[0]
RR = parms[1]
# plot the -log-posterior
a = np.arange(0.93,1.07,0.001)
R = np.arange(0.7,1.3,0.01)
Q = np.zeros(shape=(len(R),len(a)))
X,Y = np.meshgrid(a,R)
for }\textrm{n}\mathrm{ in range(0,len(a)):
    for m in range(0,len(R)):
                Q[m,n] = posteriorpdf([a[n],R[m]],sigmax/np.sqrt(Varx),sigmay/np.sqrt(Vary),rho,nn)
plt.figure(
    num=2,
    figsize=(7,5.08),
    dpi=80,
    facecolor='white')
mpl.rcParams['axes.linewidth']=2
plt.axes([0.15,0.18,0.82,0.70],
    axisbg='lightgray')
CS = plt.contourf(X,Y,Q,100)
# We draw two contour lines into the plot, the smaller of which is suitable for reading the
CS2 = plt.contour(CS,levels=[0.2,1,2,3],colors=('W','r','W', 'w'),linewidths=(2,),hold='on')
plt.clabel(CS2, inline=1, fmt='%1.1f', fontsize=16)
plt.plot(aa,RR,'wo')
plt.title('-log-posterior',fontsize=24)
```

```
plt.xlabel(r'$a\sqrt{\mathrm{Var}(x)/\mathrm{Var}(y)}$',
    fontsize=24)
plt.ylabel(r'$R/(\mathrm{Var}(x)\mathrm{Var}(y))^{1/4}$',
    fontsize=24)
cbar = plt.colorbar(CS)
cbar.ax.set_ylabel(r'$Q(a,R)$',fontsize=24)
plt.show()
# We determine the standard error of the parameters from the contour line
cc = CS2.collections[1].get_paths() [0]
CC = cc.vertices
sam = aa-min(CC[:,0])
sap = max (CC[:,0])-aa
sRm = RR-min(CC[:,1])
sRp = max (CC[:,1])-RR
print('Scaled parameters:')
print('a\' = %1.3f +%1.3f/-%1.3f'% (aa,sap,sam))
print('R\' = %1.2f +%1.2f/-%1.2f\n'% (RR,sRp,sRm))
# Calculating the slope and the intercept parameter and their errors
print('Estimated parameters:')
aest = aa*np.sqrt(Vary/Varx)
sam1 = sam*np.sqrt(Vary/Varx)
sap1 = sap*np.sqrt(Vary/Varx)
print('a = %1.3f +%1.3f/-%1.3f,% (aest,sap1,sam1))
best = Meany - Meanx*aest
bstd = np.sqrt( (sigmay*sigmay+sigmax*sigmax*aest)/nn + Meanx*Meanx*sam1*sap1)
print('b = %1.2f +/-%1.2f,% (best,bstd))
#
# Plot data with error bars and fitted line
#
x = np.arange(min(xi),max(xi),0.1)
y = aest*x + best
plt.figure(
    num=1,
    figsize=(7,5.08),
    dpi=80,
    facecolor='white')
```

```
mpl.rcParams['axes.linewidth']=2
plt.axes([0.15,0.18,0.82,0.70],
    axisbg='lightgray')
plt.errorbar(xi, yi, xerr=sigmax, yerr=sigmay, fmt='o')
plt.plot(x,y,'r',linewidth=2)
plt.axis([0,21,5,45])
plt.xticks([0,10,20],
    fontsize=24,
    fontname='Times New Roman')
plt.yticks([10, 20,30,40],
    fontsize=24,
    fontname='Times New Roman')
plt.tick_params(width=2,length=10)
plt.xlabel(r'$x$',
    fontsize=24)
plt.ylabel(r'$y$',
    fontsize=24)
plt.title('Data with errors in x and y',fontsize=24)
plt.text(2,40,r"$y = a x + b$",
    fontsize=24,
    fontname='Times New Roman')
plt.text(2,35,r"$a = 2.039\pm$",
    fontsize=24,
    fontname='Times New Roman')
plt.text(8,36.8,r"$0.076$",
    fontsize=24,
    fontname='Times New Roman')
plt.text(8,33.2,r"$0.073$",
    fontsize=24,
    fontname='Times New Roman')
plt.text(2,30,r"$b = 4.17\pm 0.83$",
    fontsize=24,
    fontname='Times New Roman')
plt.show()
```


[^0]:    ${ }^{1}$ Stephen F. Gull, Bayesian Data Analysis: Straight-line Fitting in: Maximum Entropy and Bayesian Methods, J. Skilling (ed.), (Kluwer Academic Publishers, Dordrecht, 1988), pp. 53-74.

[^1]:    ${ }^{2}$ Nuisance parameters are parameters of a model that are not of immediate interest in the analysis. Here we are aiming at the determination of $\alpha$ and $\beta$. The true positions $x_{i}$ are not of interest to us.
    ${ }^{3}$ Sir Harold Jeffreys suggested the use of this prior for (positive) scale parameters in his book Theory of Probability.

