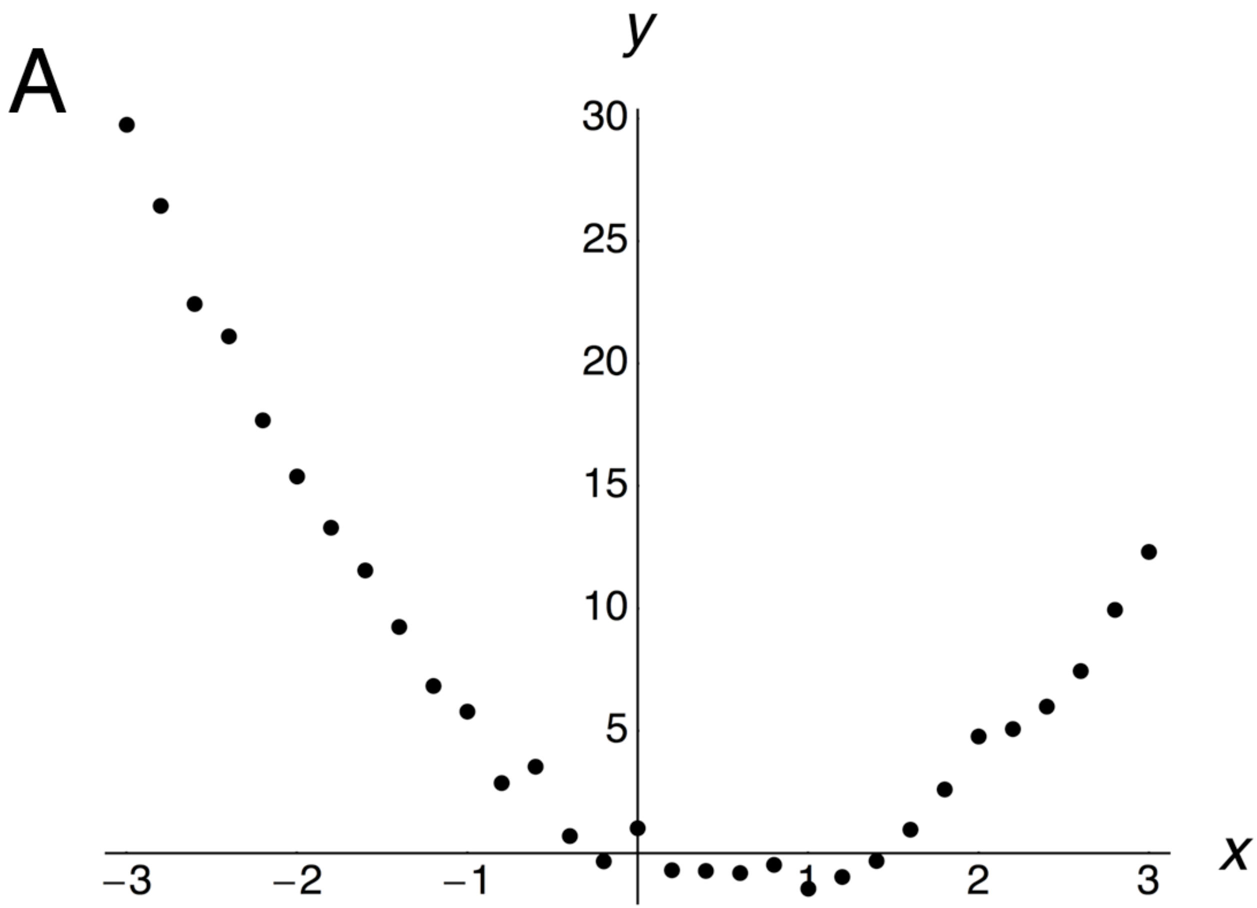

A
y
30
25
20
15
10
5
x
−3
−2
−1
1
2
3

Data

$\{x_1,\ y_1\}$

$\{x_2,\ y_2\}$

$\{x_3,\ y_3\}$

$\vdots$

$\{x_n,\ y_n\}$

Function

$$f\left(x;\ p_1,\ p_2,\ \ldots,\ p_m\right)$$
$$= f\left(x;\ \vec{p}\right)$$

Fitted values

$\{x_1,\ f(x_1)\}$

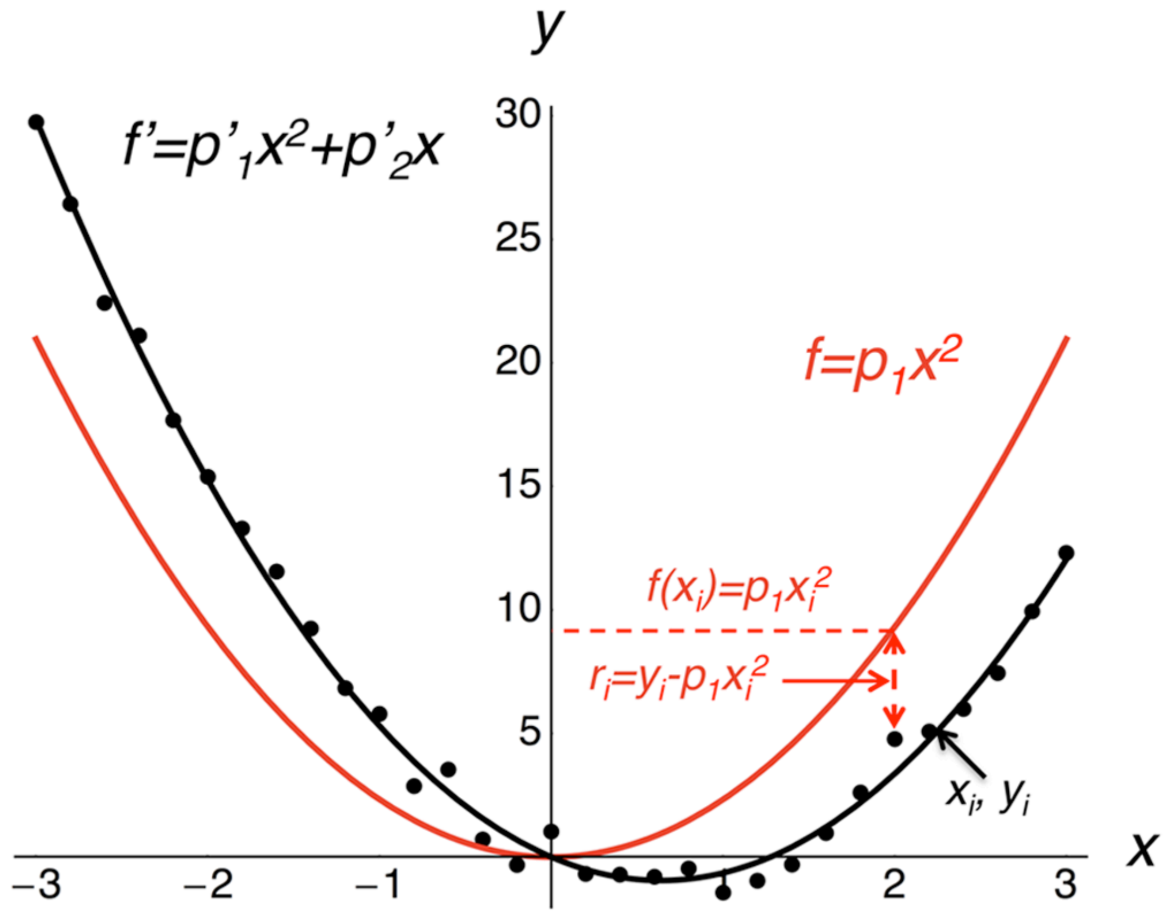
$\{x_2,\ f(x_2)\}$

$\{x_3,\ f(x_3)\}$

$\vdots$

$\{x_n,\ f(x_n)\}$

B



$f'=p'_1x^2+p'_2x$
$f=p_1x^2$
$f(x_i)=p_1x_i^2$
$r_i=y_i-p_1x_i^2$
x_i, y_i
y
x
30
25
20
15
10
5
−3
−2
−1
2
3

Things to minimize to get a good fit

Residual

$$r_i = y_i - f(x_i;\vec{p})$$

Square residuals

$$r_i^2 = \left\{ y_i - f(x_i;\vec{p}) \right\}^2$$

Sum of residuals

$$SR = \sum_{i=1}^{n} r_i$$

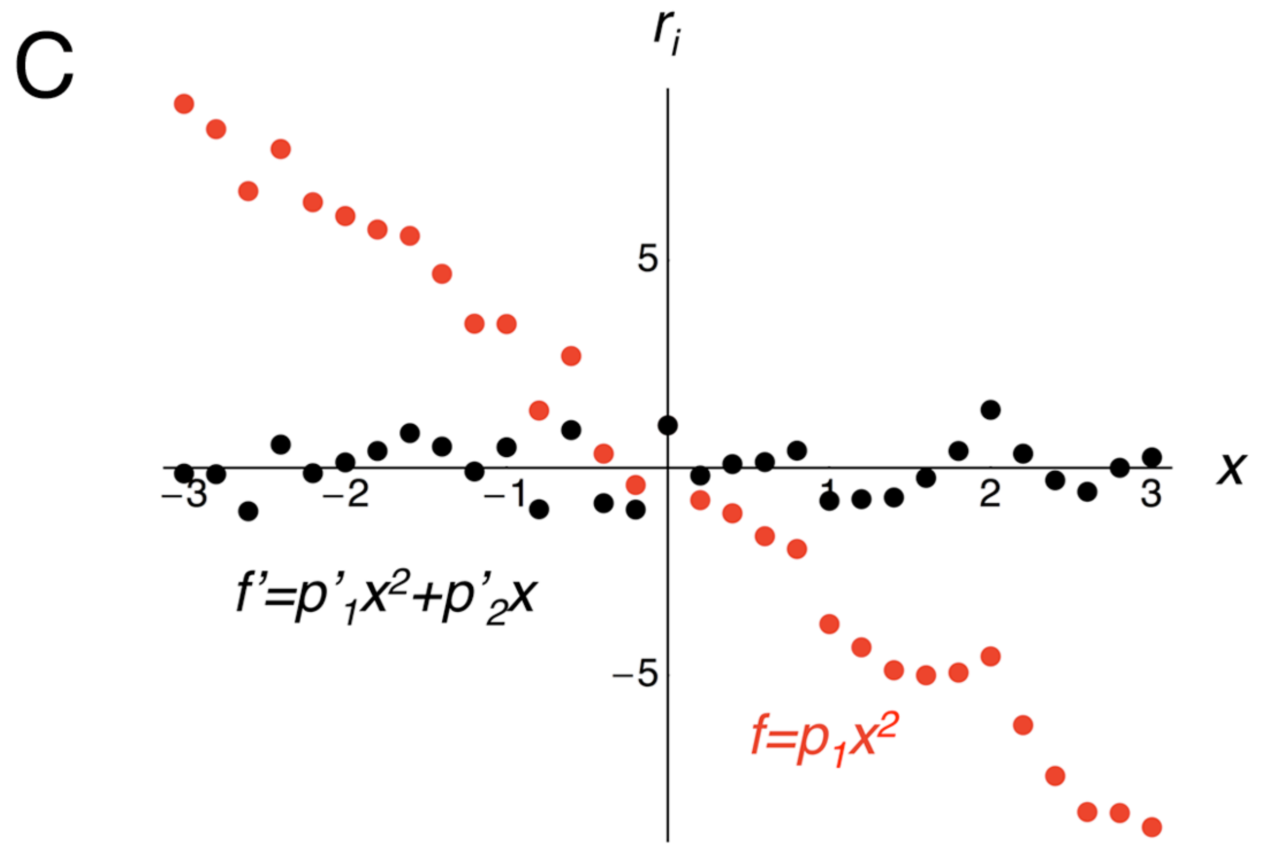
$$= \sum_{i=1}^{n} \left\{ y_i - f\left(x_i;\ \vec{p}\right) \right\}$$

Sum of square of residuals,
(*not "Chi squared"*)

$$SSR = \sum_{i=1}^{n} r_i^2$$

$$= \sum_{i=1}^{n} \left\{ y_i - f\left(x_i;\ \vec{p}\right) \right\}^2$$

The sum of residuals is already minimized!



x

Minimizing the Sum of squares of residuals (SSR)

For every parameter p_1, p_2, … p_m

$$\left(\frac{\partial SSR(\vec{p})}{\partial p_1}\right)_{p\neq p_1} = 0$$

$$\left(\frac{\partial SSR(\vec{p})}{\partial p_2}\right)_{p\neq p_2} = 0$$

$$\vdots$$

$$\left(\frac{\partial SSR(\vec{p})}{\partial p_m}\right)_{p\neq p_m} = 0$$

As a single variation equation:

$$\begin{aligned} d(SSR) &= \sum_{j=1}^{m}\left(\frac{\partial SSR}{\partial p_j}\right)_{p_{k\neq j}} dp_j \\ &= \sum_{j=1}^{m}\frac{\partial}{\partial p_j}\left(\sum_{i=1}^{n}\left\{y_i - f\left(x_i;\ \vec{p}\right)\right\}^2\right)dp_j \\ &= -\sum_{j=1}^{m}\left(\sum_{i=1}^{n}2\left\{y_i - f\left(x_i;\ \vec{p}\right)\right\}\frac{\partial f\left(x_i;\ \vec{p}\right)}{\partial p_j}\right)_{p_{k\neq j}} dp_j = 0 \end{aligned}$$

$$0 = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\left\{y_i - f\left(x_i;\ \vec{p}_{best}\right)\right\}\frac{\partial f\left(x_i;\ \vec{p}_{best}\right)}{\partial p_j}\right)_{p_{k\neq j}} dp_j$$

$$0 = \left(\sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f_i}{\partial p_1}\right)dp_1 \qquad \sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f\left(x_i;\ \vec{p}_{best}\right)}{\partial p_1} = 0$$

$$0 = \left(\sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f_i}{\partial p_2}\right)dp_2 \quad \xrightarrow{dp_2 \neq 0} \quad \sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f\left(x_i;\ \vec{p}_{best}\right)}{\partial p_2} = 0$$

$$\vdots \qquad\qquad\qquad \vdots$$

$$0 = \left(\sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f_i}{\partial p_m}\right)dp_m \qquad \sum_{i=1}^{n}\left\{y_i - f_i\right\}\frac{\partial f\left(x_i;\ \vec{p}_{best}\right)}{\partial p_m} = 0$$

Least-squares for linear models:

$$f(x,\vec{p}) = p_1 g_1(x) + p_2 g_2(x) + \ldots + p_m g_m(x)$$

$$\left(\frac{\partial f\left(x_i;\ \vec{p}\right)}{\partial p_j}\right)_{p_{k\neq j}} = g_j(x_i) \quad \Longrightarrow \quad \begin{aligned} \sum_{i=1}^{n} f_i g_1(x_i) &= \sum_{i=1}^{n} (y_i) g_1(x_i) \\ \sum_{i=1}^{n} f_i g_2(x_i) &= \sum_{i=1}^{n} (y_i) g_2(x_i) \\ &\vdots \\ \sum_{i=1}^{n} f_i g_m(x_i) &= \sum_{i=1}^{n} (y_i) g_m(x_i) \end{aligned}$$

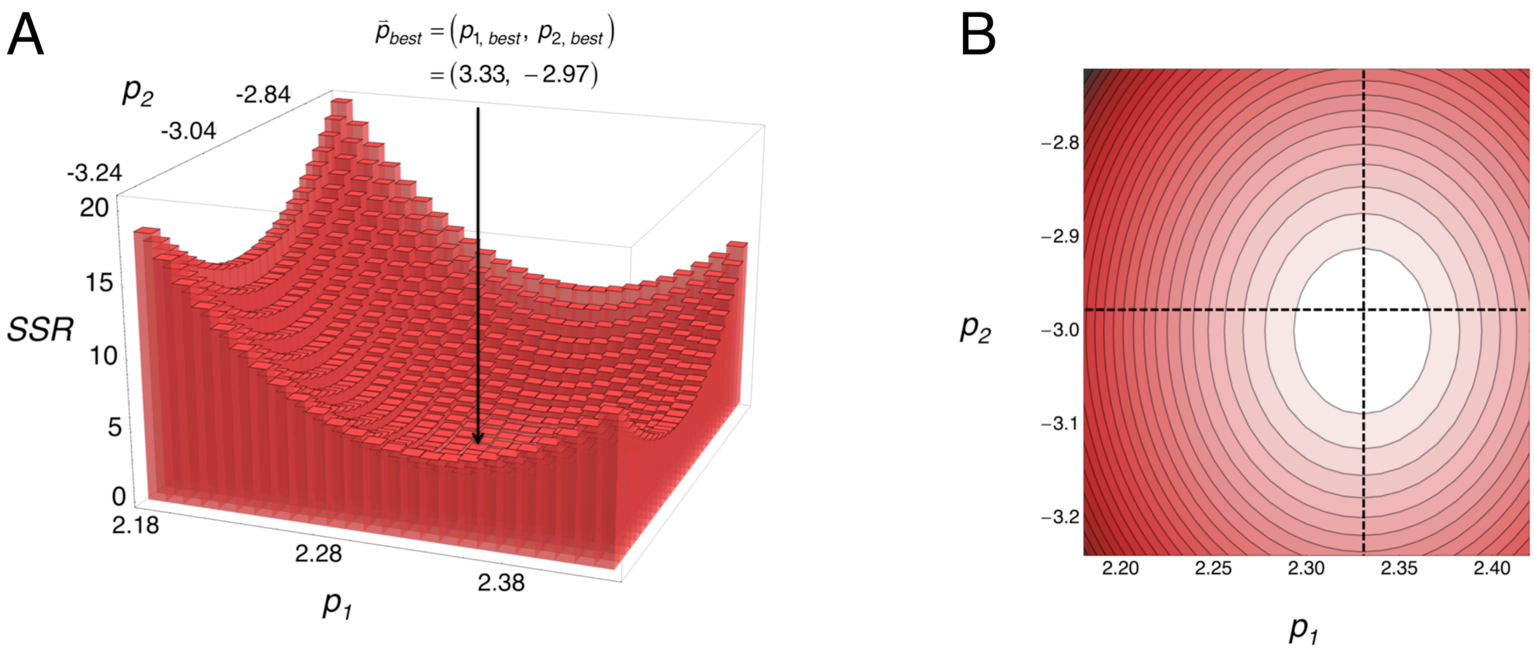
Expanding f(x, p),

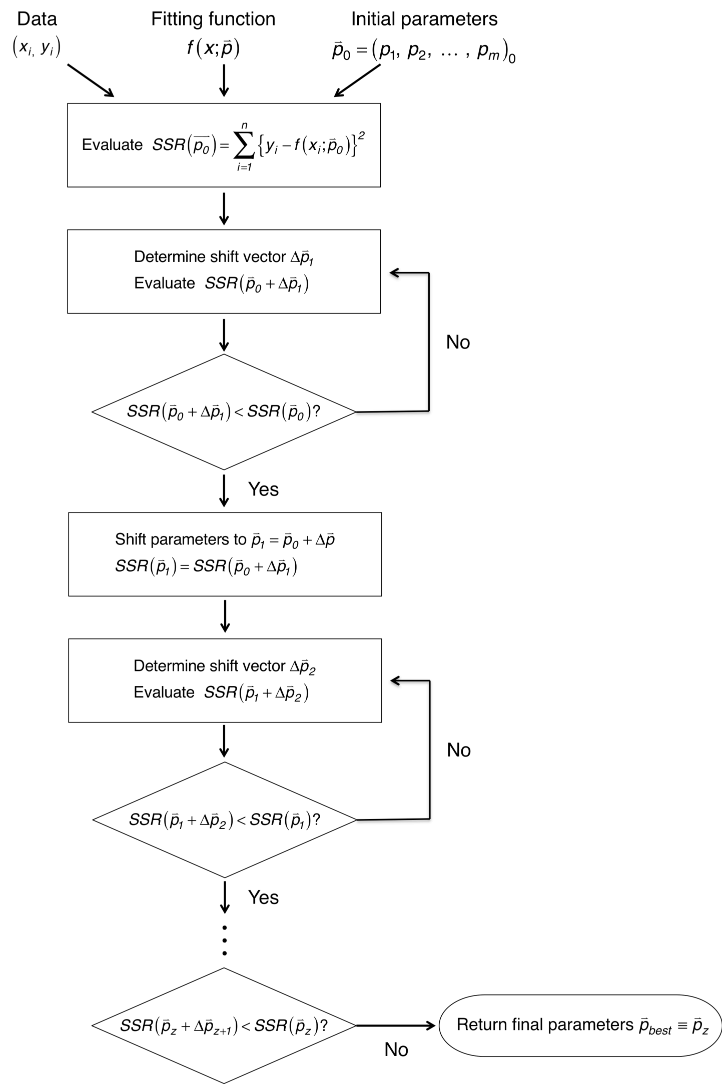
$$\begin{aligned} p^*{}_1 \sum_{i=1}^{n} g_1(x_i)^2 + p^*{}_2 \sum_{i=1}^{n} g_2(x_i) g_1(x_i) + \cdots + p^*{}_m \sum_{i=1}^{n} g_m(x_i) g_1(x_i) &= \sum_{i=1}^{n} y_i g_1(x_i) \\ p^*{}_1 \sum_{i=1}^{n} g_1(x_i) g_2(x_i) + p^*{}_2 \sum_{i=1}^{n} g_2(x_i)^2 + \cdots + p^*{}_m \sum_{i=1}^{n} g_m(x_i) g_2(x_i) &= \sum_{i=1}^{n} y_i g_2(x_i) \\ &\vdots \\ p^*{}_1 \sum_{i=1}^{n} g_1(x_i) g_m(x_i) + p^*{}_2 \sum_{i=1}^{n} g_2(x_i) g_m(x_i) + \cdots + p^*{}_m \sum_{i=1}^{n} g_m(x_i)^2 &= \sum_{i=1}^{n} y_i g_m(x_i) \end{aligned}$$

$$
\begin{bmatrix}
\sum_{i=1}^{n} g_1(x_i)^2 & \sum_{i=1}^{n} g_2(x_i)g_1(x_i) & \cdots & \sum_{i=1}^{n} g_m(x_i)g_1(x_i) \\
\sum_{i=1}^{n} g_1(x_i)g_2(x_i) & \sum_{i=1}^{n} g_2(x_i)^2 & \cdots & \sum_{i=1}^{n} g_m(x_i)g_2(x_i) \\
\vdots & & & \\
\sum_{i=1}^{n} g_1(x_i)g_m(x_i) & \sum_{i=1}^{n} g_2(x_i)g_m(x_i) & \cdots & \sum_{i=1}^{n} g_m(x_i)^2
\end{bmatrix}
\begin{bmatrix} p^{*}_{1} \\ p_2^{*} \\ \vdots \\ p_m^{*} \end{bmatrix}
=
\begin{bmatrix} \sum_{i=1}^{n} y_i g_1(x_i) \\ \sum_{i=1}^{n} y_i g_2(x_i) \\ \vdots \\ \sum_{i=1}^{n} y_i g_m(x_i) \end{bmatrix}
$$

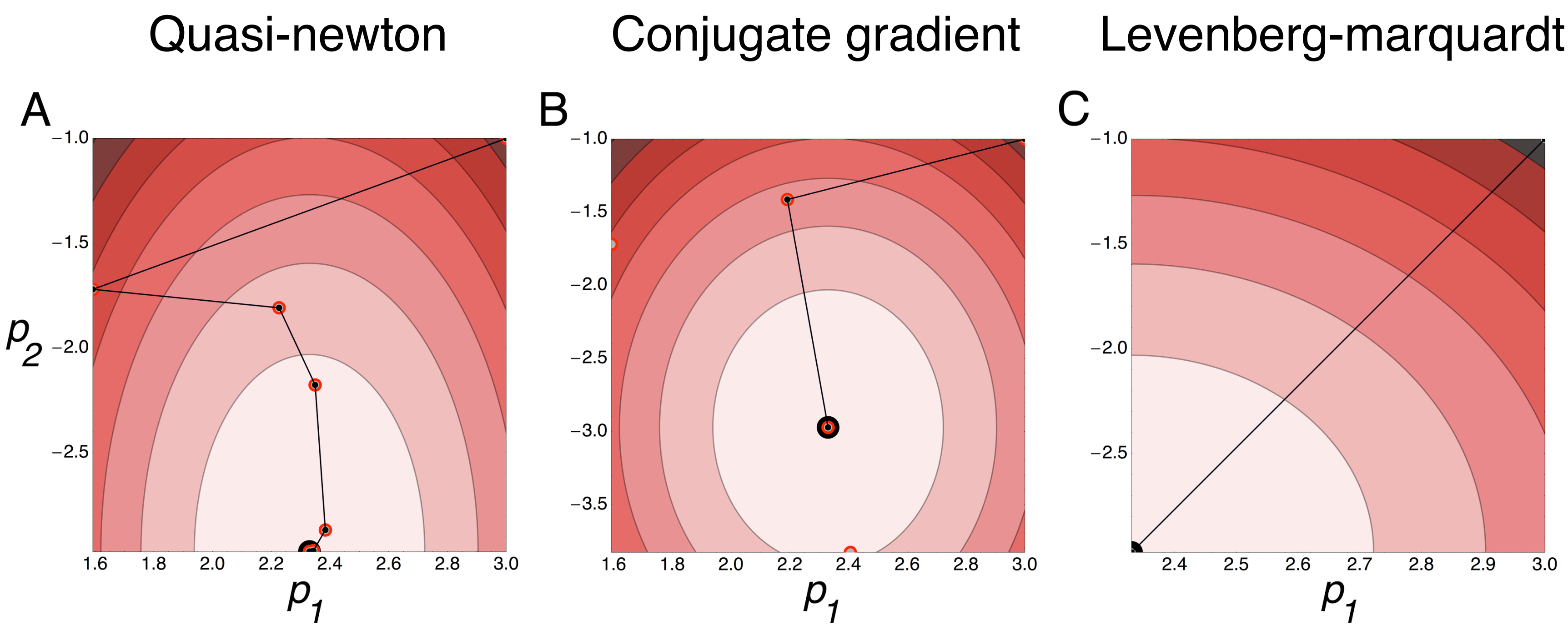
$$
\begin{bmatrix}
\sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_1}\right)^2 & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_1}\right)\left(\frac{\partial f_i}{\partial p_2}\right) & \cdots & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_1}\right)\left(\frac{\partial f_i}{\partial p_m}\right) \\
\sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_1}\right)\left(\frac{\partial f_i}{\partial p_2}\right) & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_2}\right)^2 & \cdots & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_2}\right)\left(\frac{\partial f_i}{\partial p_m}\right) \\
\vdots & & & \\
\sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_1}\right)\left(\frac{\partial f_i}{\partial p_m}\right) & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_2}\right)\left(\frac{\partial f_i}{\partial p_m}\right) & \cdots & \sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial p_m}\right)^2
\end{bmatrix}
\begin{bmatrix} p^{*}_{1} \\ p_2^{*} \\ \vdots \\ p_m^{*} \end{bmatrix}
=
\begin{bmatrix} \sum_{i=1}^{n} y_i \left(\frac{\partial f_i}{\partial p_1}\right) \\ \sum_{i=1}^{n} y_i \left(\frac{\partial f_i}{\partial p_2}\right) \\ \vdots \\ \sum_{i=1}^{n} y_i \left(\frac{\partial f_i}{\partial p_m}\right) \end{bmatrix}
$$

$$Y=p_1x^2+p_2x$$


A
$\vec{p}_{best} = (p_{1,\,best},\ p_{2,\,best})$
$= (3.33,\ -2.97)$
p_2
-2.84
-3.04
-3.24
20
15
SSR
10
5
0
2.18
2.28
2.38
p_1
B
−2.8
−2.9
p_2
−3.0
−3.1
−3.2
2.20
2.25
2.30
2.35
2.40
p_1

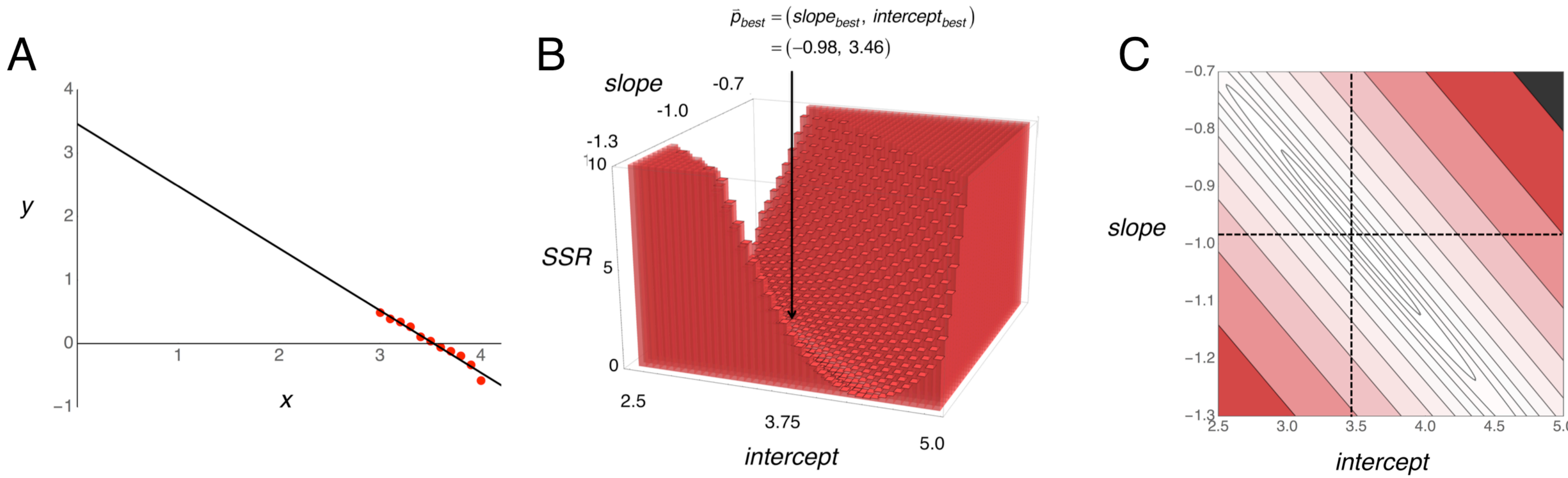

Data
(x_i, y_i)
Fitting function
$f(x;\vec{p})$
Initial parameters
$\vec{p}_0 = (p_1, p_2, \dots, p_m)_0$
Evaluate $SSR(\overline{p_0}) = \sum_{i=1}^{n} \{y_i - f(x_i;\vec{p}_0)\}^2$
Determine shift vector $\Delta\vec{p}_1$
Evaluate $SSR(\vec{p}_0 + \Delta\vec{p}_1)$
$SSR(\vec{p}_0 + \Delta\vec{p}_1) < SSR(\vec{p}_0)$?
No
Yes
Shift parameters to $\vec{p}_1 = \vec{p}_0 + \Delta\vec{p}$
$SSR(\vec{p}_1) = SSR(\vec{p}_0 + \Delta\vec{p}_1)$
Determine shift vector $\Delta\vec{p}_2$
Evaluate $SSR(\vec{p}_1 + \Delta\vec{p}_2)$
$SSR(\vec{p}_1 + \Delta\vec{p}_2) < SSR(\vec{p}_1)$?
No
Yes
$SSR(\vec{p}_z + \Delta\vec{p}_{z+1}) < SSR(\vec{p}_z)$?
No
Return final parameters $\vec{p}_{best} \equiv \vec{p}_z$

$$Y=p_1x^2+p_2x$$



Little red circles—evaluate chi squared
Grey circles—evaluate its gradient
Big black circle--minimum

$$Y = p_1 x + p_2$$


A
B
C
$\vec{p}_{best} = (slope_{best},\ intercept_{best}) = (-0.98,\ 3.46)$
x
y
slope
SSR
intercept

Covariance matrix

$$V = \begin{bmatrix} V_{1,1} & V_{2,1} & \cdots & V_{m,1} \\ V_{1,2} & V_{2,2} & & \\ \vdots & & \ddots & \\ V_{1,m} & & & V_{m,m} \end{bmatrix}$$

$$s_{p_i} = V_{i,i}^{\ 1/2}$$

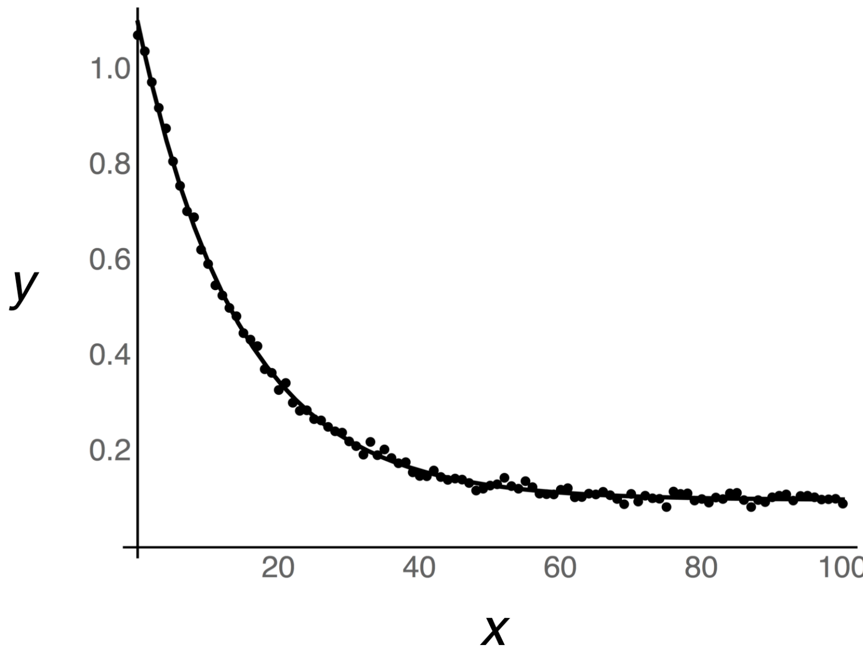
Correlation matrix

$$C = \begin{bmatrix} C_{1,1} & C_{2,1} & \cdots & C_{m,1} \\ C_{1,2} & C_{2,2} & & \\ \vdots & & \ddots & \\ C_{1,m} & & & C_{m,m} \end{bmatrix}$$

$$C_{i,j} = \frac{V_{i,j}}{V_{i,i}^{\ 1/2} \times V_{j,j}^{\ 1/2}}$$

A nonlinear fit

$$f(x) = (y_0 - y_\infty)e^{-kx} + y_\infty$$



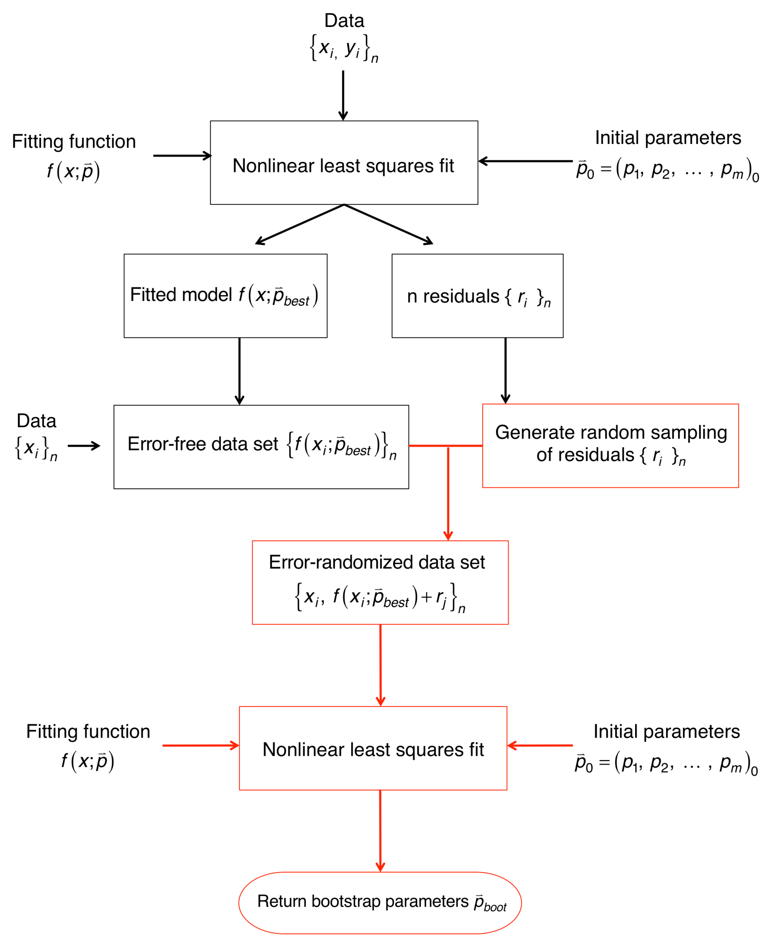
$y_\infty = 0.0998 \quad y_0 = 1.100 \quad k = 0.0697$

$s_{y_\infty} = 0.0014 \quad s_{y_0} = 0.0049 \quad s_k = 0.00062$

$$V = \begin{bmatrix} 2.07\times10^{-6} & 1.76\times10^{-6} & 5.52\times10^{-7} \\ 1.76\times10^{-6} & 2.39\times10^{-5} & 2.03\times10^{-6} \\ 5.52\times10^{-7} & 2.03\times10^{-6} & 3.80\times10^{-7} \end{bmatrix}$$

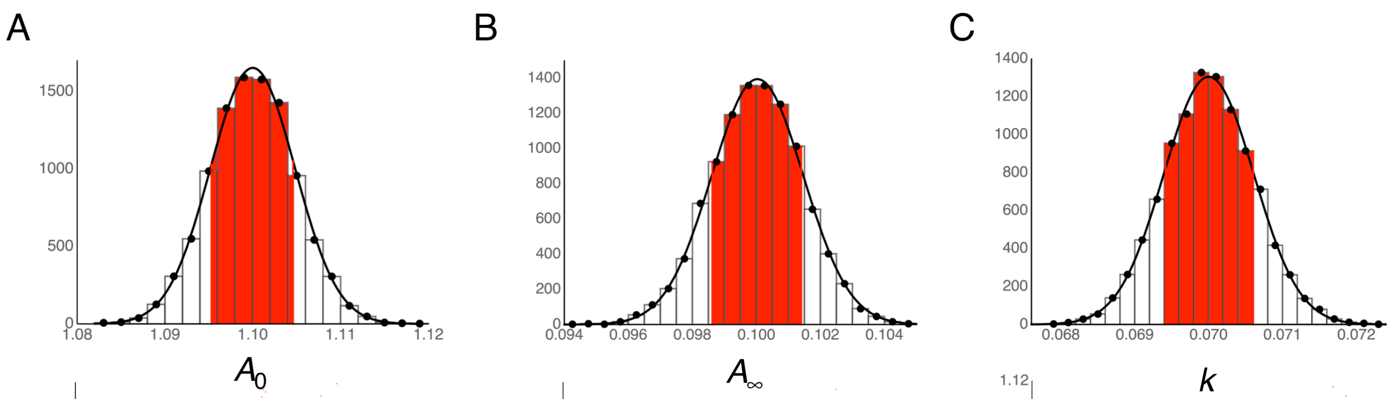
$$C = \begin{bmatrix} 1 & 0.250 & 0.622 \\ 0.250 & 1 & 0.673 \\ 0.622 & 0.673 & 1 \end{bmatrix}$$

The bootstrap method



The bootstrap for the exponential decay

10,000 iterations



$C(A_0, A_\infty) = 0.250$ $\quad$ $C(k, A_\infty) = 0.622$ $\quad$ $C(A_0, k) = 0.673$

Table 2.1. Estimates of parameter uncertainty from the exponential decay fit.

Parameter	Best fit value	Uncertainty from covariance matrix	Bootstrap standard deviation	Bootstrap 67% confidence intervals	*f*-statistic 67% confidence intervals
y_0	1.0999	0.00489	0.00479	1.0953, 1.1046	1.084, 1.116
y_∞	0.0998	0.00144	0.00142	0.0986, 0.1014	0.0984, 0.1012
k	0.0697	0.000616	0.00061	0.06941, 0.07061	0.0677, 0.0717

The data set and fit is from Figure 2.18. The uncertainty from the covariance matrix is from equation 2.76. Bootstrap analysis was performed as in Figure 2.19, with 10,000 iterations (Figure 2.20). Confidence intervals from *f*-statistics were determined as illustrated in Figures 2.21 and 2.22.

Does a single model fit well? The probability distribution for chi-squared.

$$\chi^2 = \frac{1}{\sigma_y^2}\sum_{i=1}^{n}\left(y_i - f\left(x_i\right)\right)^2 = \frac{SSR}{\sigma_y^2}$$

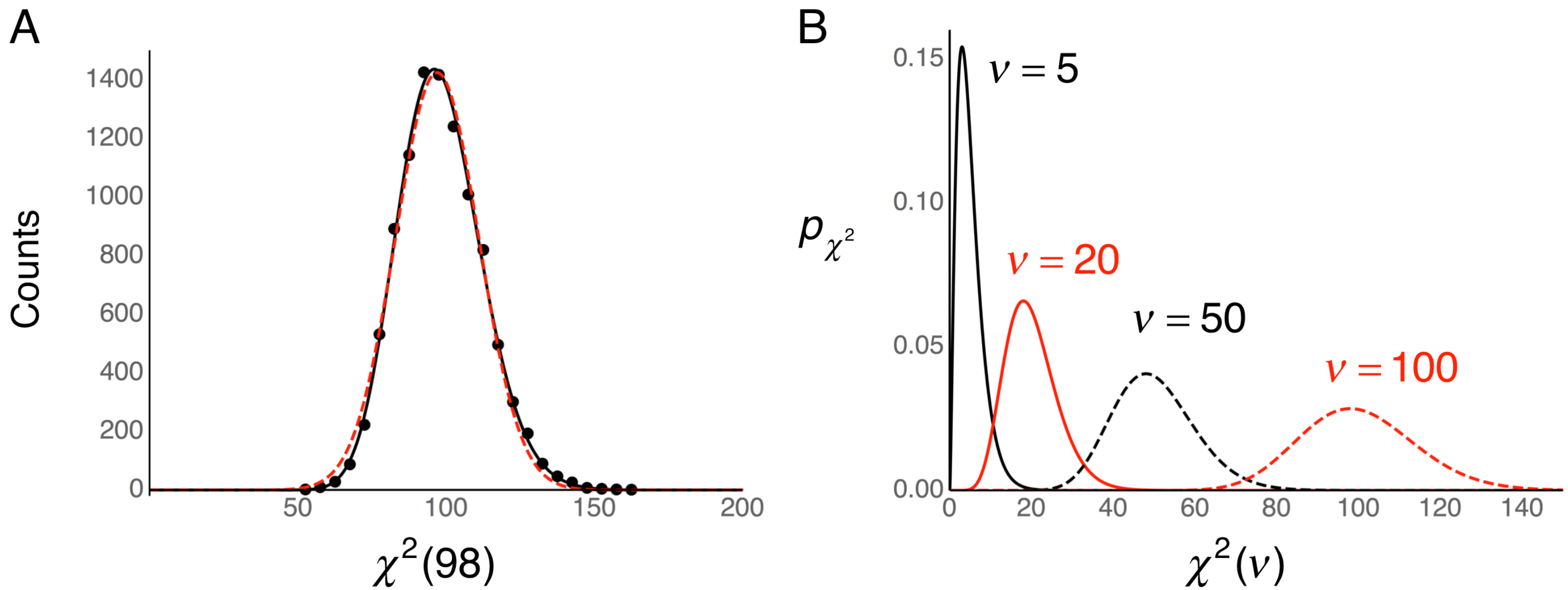
$$\chi_r^2 = \frac{\chi^2}{\nu} = \frac{1}{(n-m)\sigma_y^2}\sum_{i=1}^{n}\left(y_i - f\left(x_i\right)\right)^2 = \frac{MSR}{\sigma_y^2}$$

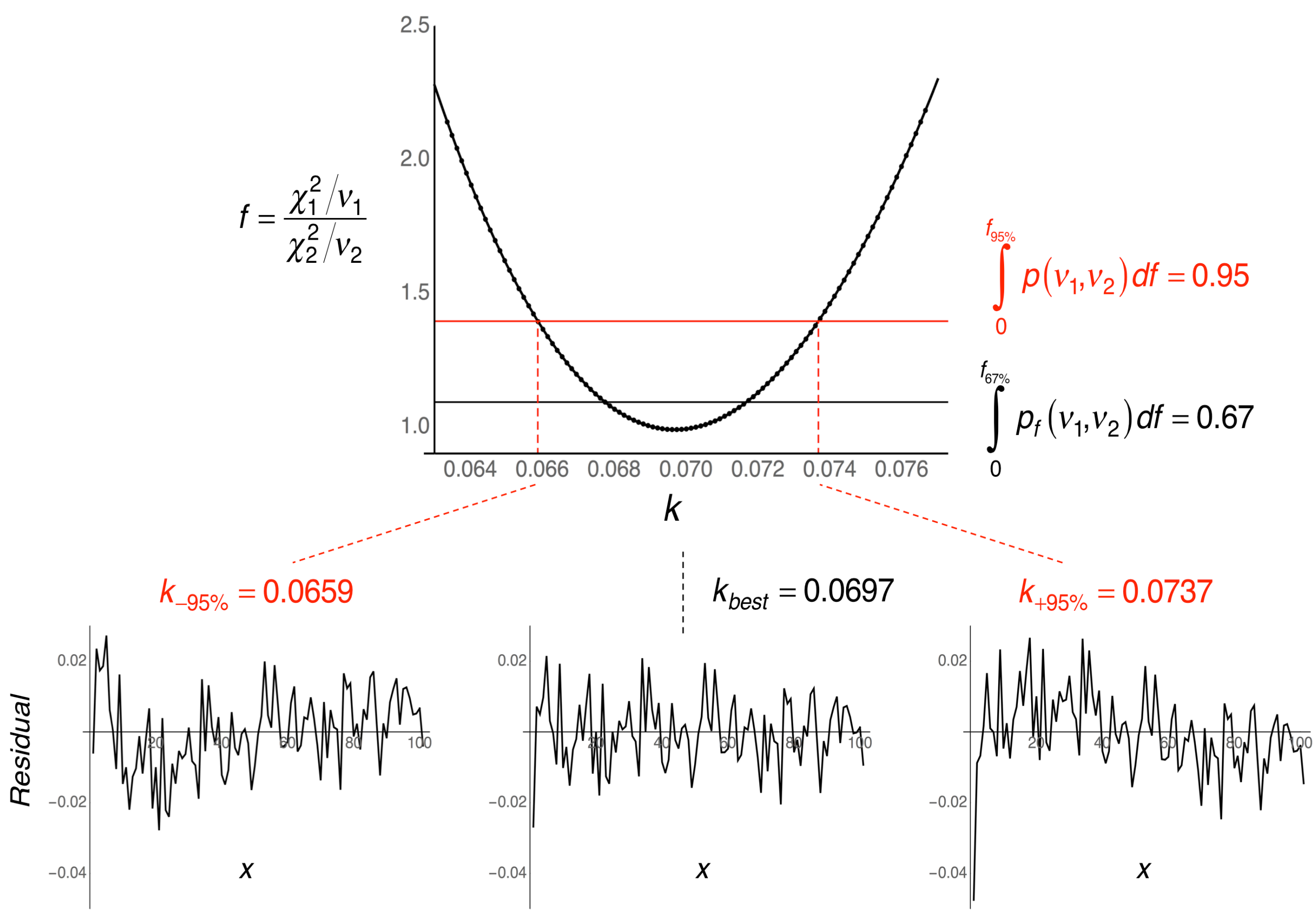
Chi Squared distribution

$$p_{\chi^2} = \frac{\left(\chi^2\right)^{(\nu-2)/2} e^{-\chi^2/2}}{2^{\nu/2}\Gamma(\nu/2)}$$

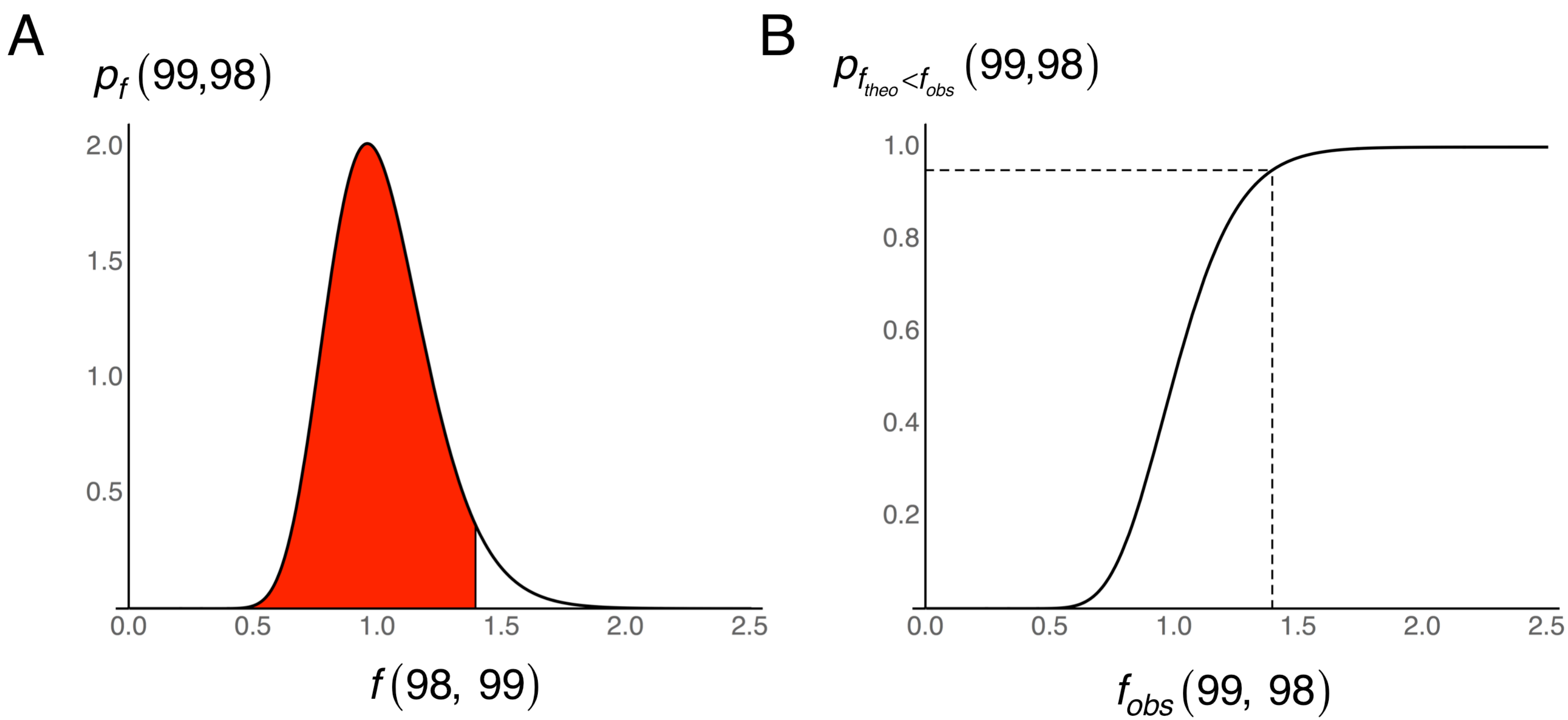
$$\Gamma(\nu) = \int_0^\infty x^{\nu-1} e^{-x}\,dx$$

$$\Gamma(\nu) = \begin{cases} (\nu-1)! = \dfrac{\nu!}{\nu} & \nu = 0,\ 1,\ 2,\ \ldots \\ (\nu-1)(\nu-2)\ldots\left(\dfrac{3}{2}\right)\left(\dfrac{\sqrt{\pi}}{2}\right) & \nu = \dfrac{1}{2},\ \dfrac{3}{2},\ \dfrac{5}{2},\ \ldots \end{cases}$$





2.5
2.0
1.5
1.0
0.064 0.066 0.068 0.070 0.072 0.074 0.076
k
$f = \dfrac{\chi_1^2 / \nu_1}{\chi_2^2 / \nu_2}$
$\int_0^{f_{95\%}} p(\nu_1,\nu_2)\,df = 0.95$
$\int_0^{f_{67\%}} p_f(\nu_1,\nu_2)\,df = 0.67$
$k_{-95\%} = 0.0659$
$k_{best} = 0.0697$
$k_{+95\%} = 0.0737$
Residual
0.02
−0.02
−0.04
20 40 60 80 100
x



A
$p_f\,(99,98)$
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
$f\,(98,\ 99)$
B
$p_{f_{theo}<f_{obs}}\,(99,98)$
1.0
0.8
0.6
0.4
0.2
0.0
0.5
1.0
1.5
2.0
2.5
$f_{obs}\,(99,\ 98)$