2021

Nonlinear statistical models

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Linear vs. nonlinear models

Linear model

$$Y = X\theta + \varepsilon$$

Nonlinear model

$$Y = f(X, \theta) + \varepsilon$$

Find θ minimizing: $OLS = Z(\theta) = \sum_{i=1}^{N} [y_i - f(x_i; \theta)]^2$

Difficulties:

non linear model

no analytical expression for the estimators

Find θ minimizing: $OLS = Z(\theta) = \sum_{i=1}^{N}[y_i - f(x_i;\theta)]^2$

For a linear model, the solution is known (computed with the R function `lm`:

$$Y = X\theta + \varepsilon$$

$$\hat{\theta} = (X'X)^{-1}X'Y$$

Find θ minimizing: $OLS = Z(\theta) = \sum_{i=1}^{N}[y_i - f(x_i; \theta)]^2$

For a linear model, the solution is known (computed with the R function `lm`:

$$Y = X\theta + \varepsilon$$

$$\hat{\theta} = (X'X)^{-1}X'Y$$

For a nonlinear model, the solution is unknown and needs to be approximated iteratively

Linearization of a nonlinear model

$$f\left(x;\theta\right)=e^{\theta x}$$

- Taylor expansion at a specific parameter value

$$f\left(x;\theta\right)\approx f\left(x;\hat{\theta}_0\right)+\left.\frac{df\left(x;\theta\right)}{d\theta}\right|_{\hat{\theta}_0}\left(\theta-\hat{\theta}_0\right)$$

- The model can be approximated by $A + B\ \theta$

Linearization of a nonlinear model

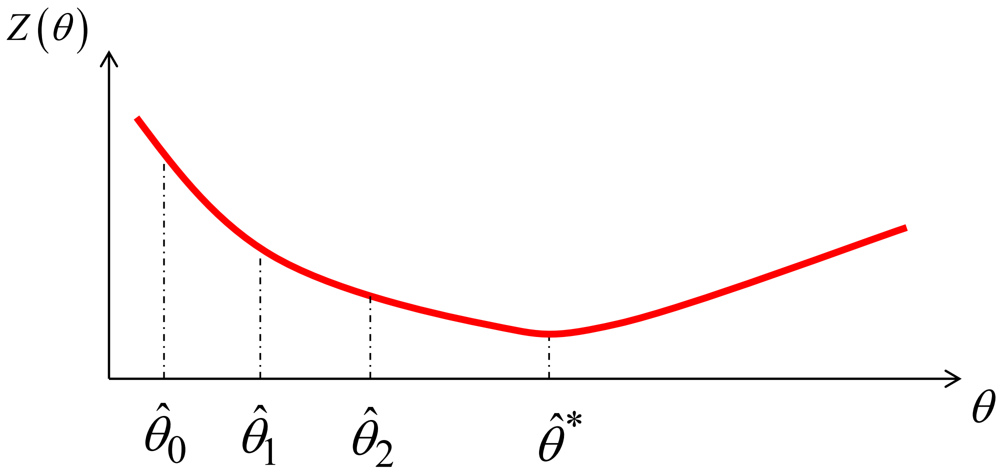
$$f(x;\theta) = e^{\theta x}$$

$$e^{\theta x} \approx e^{\hat{\theta}_0 x} + \left(\theta - \hat{\theta}_0\right) x e^{\hat{\theta}_0 x}$$

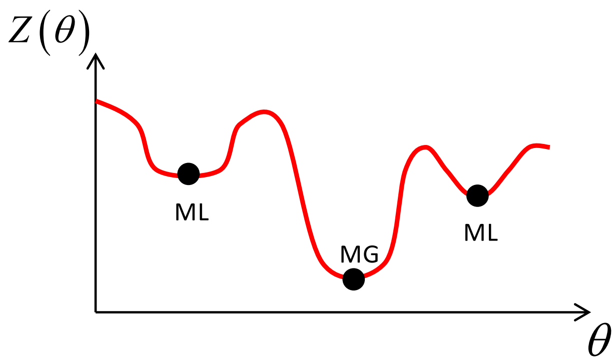
$$e^{\theta x} \approx e^{\hat{\theta}_0 x} - \hat{\theta}_0 x e^{\hat{\theta}_0 x} + x e^{\hat{\theta}_0 x} \times \theta$$

Estimator: $$\hat{\theta}_1 = \hat{\theta}_0 + \frac{\sum_{i=1}^{N} x_i e^{\hat{\theta}_0 x_i}\left(Y_i - e^{\hat{\theta}_0 x_i}\right)}{\sum_{i=1}^{N} x_i^2 e^{2\hat{\theta}_0 x_i}}$$

Minimization using an iterative algorithm



Local optimum, global optimum



→ Try several starting values!

Main steps for the development of a model

- Definition of inputs X and outputs Y
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- Tests and model assessment
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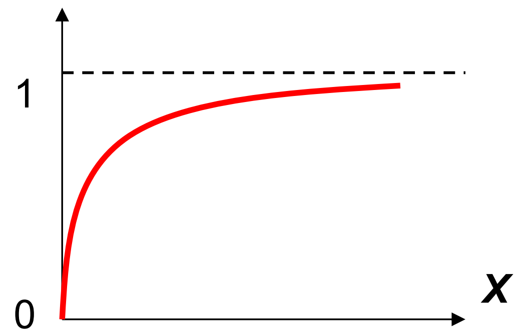
A simple example

- Non linear model predicting relative yield as a function of a factor *x* (amount of soil mineral N)

$$f(x,\theta)=\left[1-\exp\left(-\theta\times x\right)\right]$$



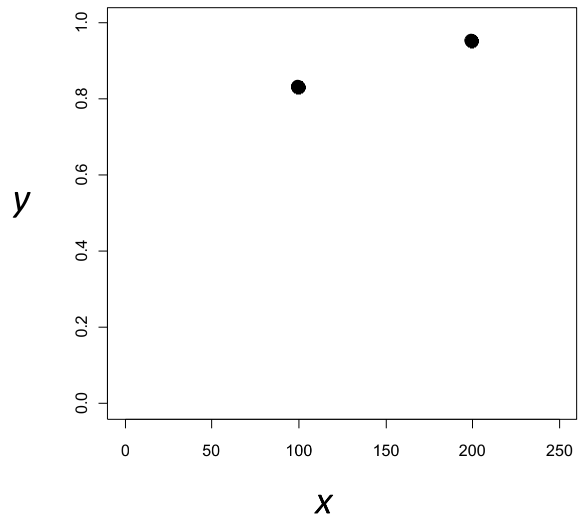
- One parameter θ → the growth rate

Data

Two measurements of relative yield y_1 and y_2 are available:

$y_1 = 0.83$ for $x_1 = 100$ kg/ha

$y_2 = 0.95$ for $x_2 = 200$ kg/ha



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Give the expression of $Z(\theta)$ in this case

$$Z(\theta)=\sum_{i=1}^{N}[y_i - f(x_i;\theta)]^2$$

Practical considerations

- Several packages were developed to implement this kind of algorithm (R, Python…)

- They use the following entries:
  i. data
  ii. a model equation,
  iii. initial parameter values.

- The output is a set of estimated parameter values.

```
x<-c(100, 200)

y<-c(0.83, 0.95)

TAB<-data.frame(x,y)
```

```
x<-c(100, 200)

y<-c(0.83, 0.95)

TAB<-data.frame(x,y)

Fit<-nls(y~1-exp(-Theta*x), data=TAB, start=list(Theta=0.05),
trace=T)

print(summary(Fit))
```

```
> Fit<-nls(y~1-exp(-Theta*x), data=TAB, start=list(Theta=0.05), trace=T)
0.02914996 :  0.05
0.001751208 :  0.01959284
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0.0003974661 :  0.01733614
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> print(summary(Fit))

Formula: y ~ 1 - exp(-Theta * x)

Parameters:
          Estimate   Std. Error   t value Pr(>|t|)
Theta     0.017336   0.001064   16.29    0.039 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01994 on 1 degrees of freedom

Number of iterations to convergence: 6
```
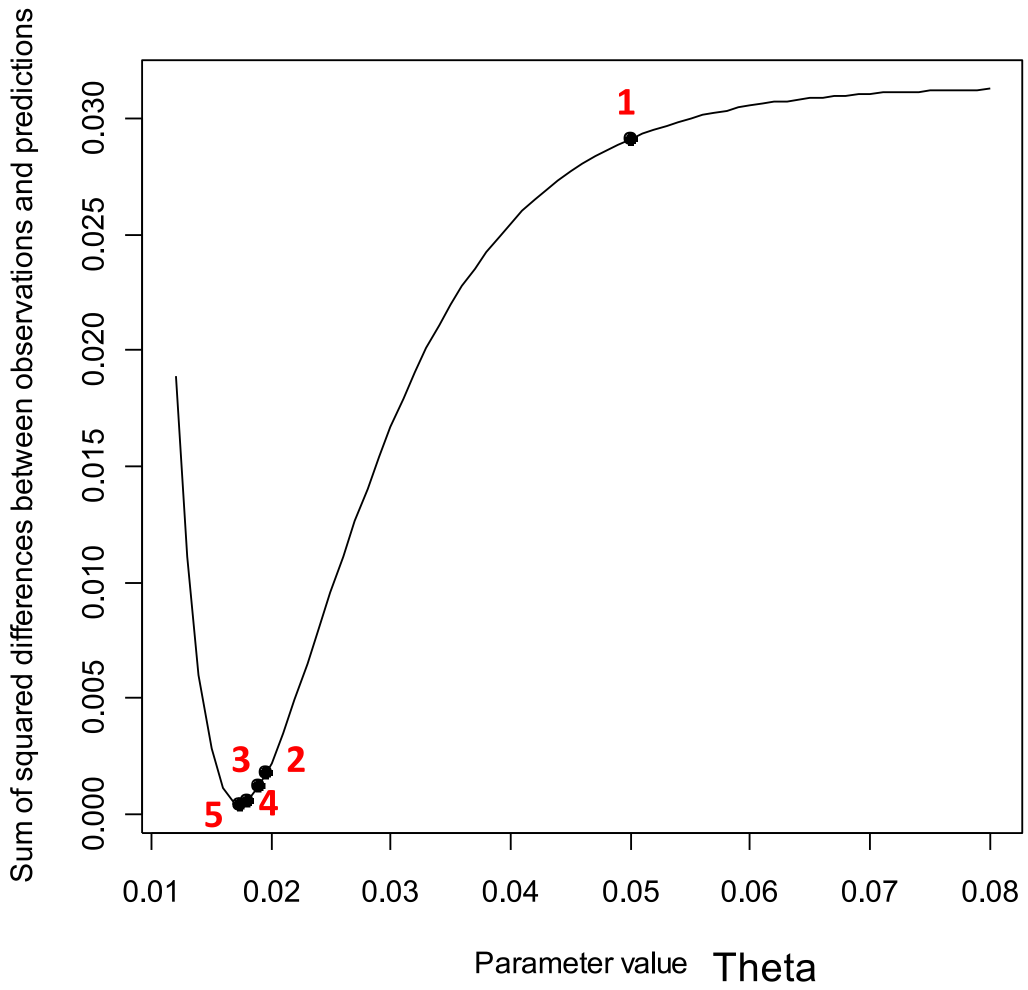
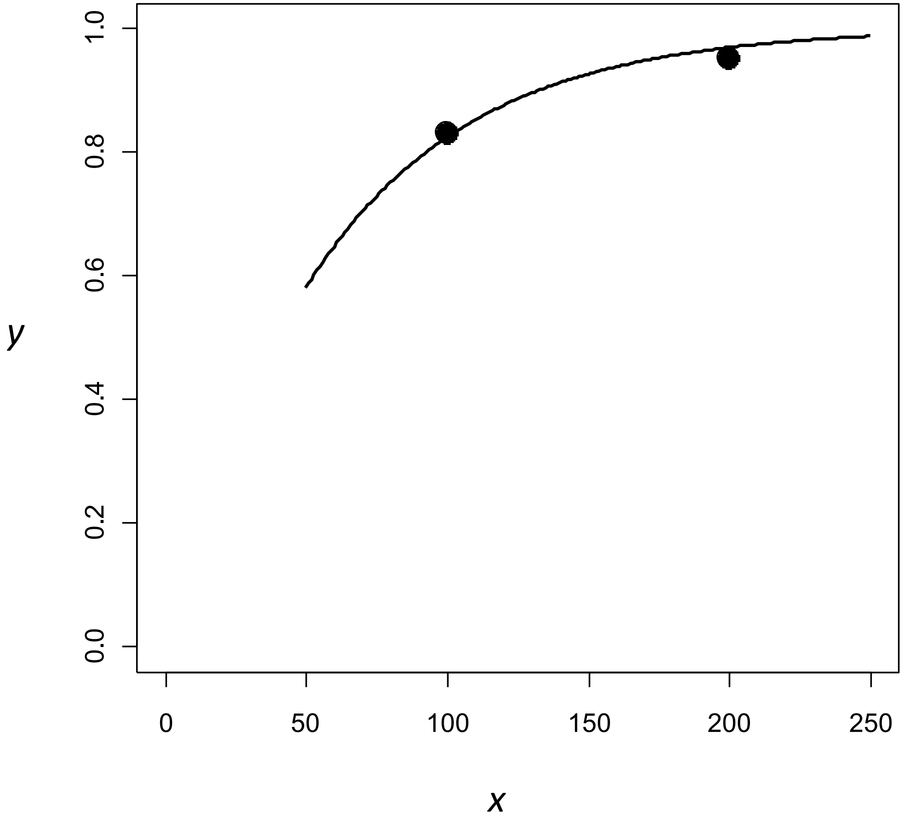

OLS (Z)



Sum of squared differences between observations and predictions
0.000
0.005
0.010
0.015
0.020
0.025
0.030
1
2
3
4
5
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
Parameter value
Theta

```
X.vec<-50:250

Y.vec<-1-exp(-coef(Fit)[1]*X.vec)

plot(x,y, xlim=c(0, 250), pch=19, cex=2, ylim=c(0,1))

lines(X.vec, Y.vec, lwd=2)
```

$\hat{\theta} = 0.0173$



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Standard error of the estimator

Estimated value of the parameter

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Standard error of the estimator

Estimate/SE

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What is the conclusion here?

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Minimum value of OLS divided by the number of data -1

=RMSE

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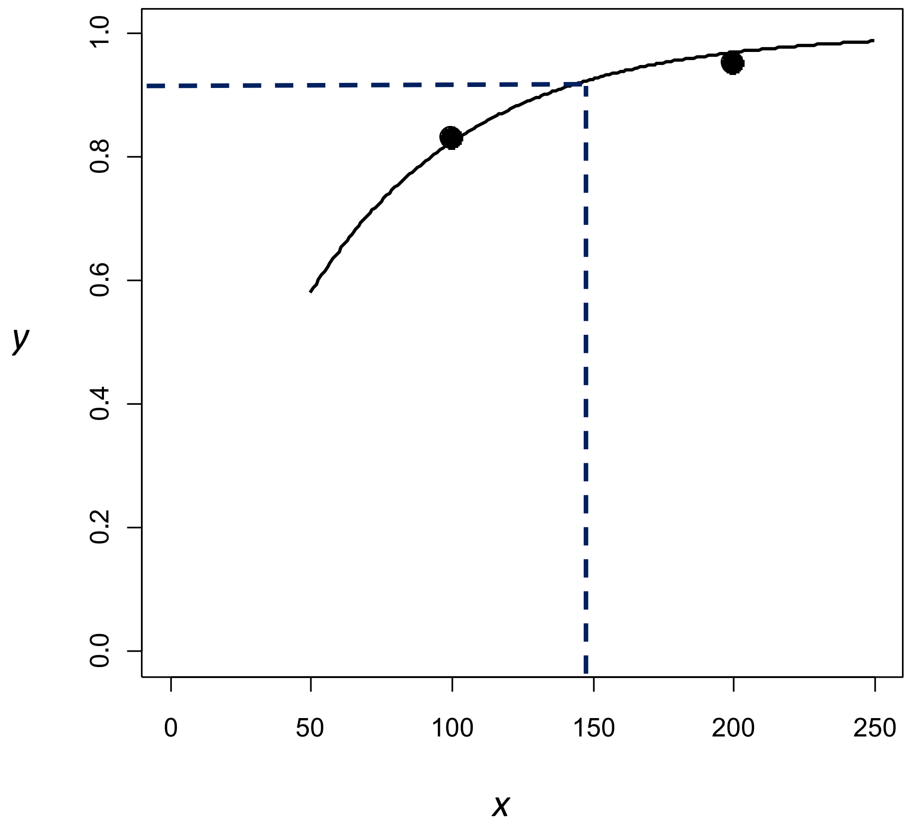
Perform uncertainty and sensitivity analysis!

$\hat{\theta} = 0.0173$

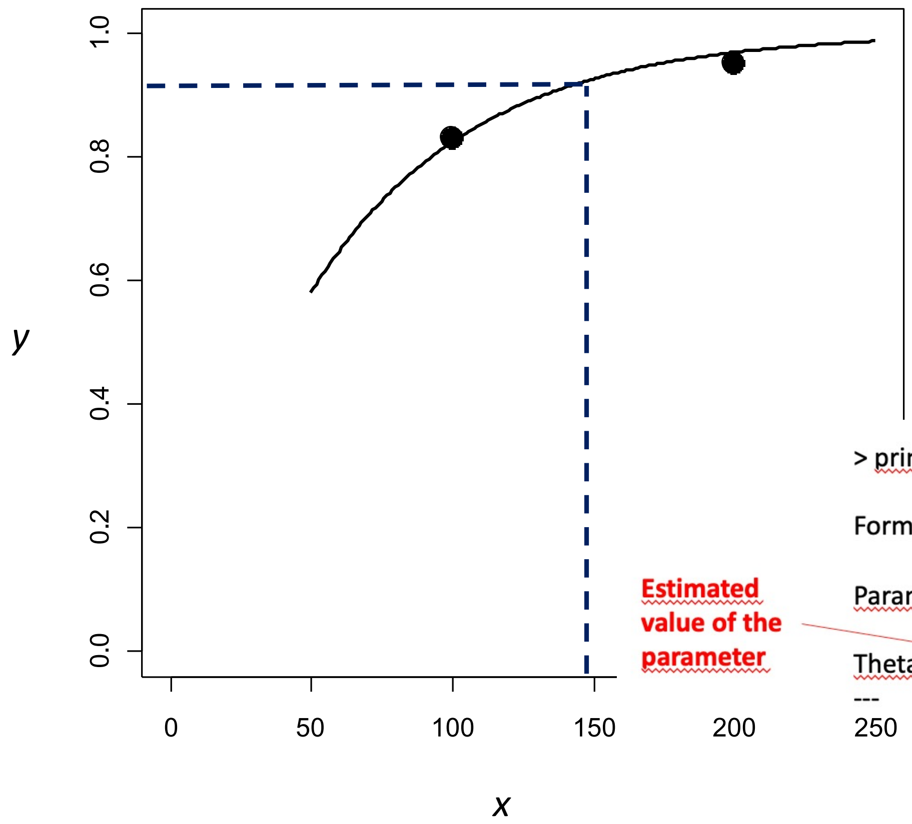
What is the value of *y* for *x*=150?



1-exp(-0.0173*150)=0.925

$\hat{\theta}$ = 0.0173

What is the value of *y* for *x*=150?



1-exp(-0.0173*150)=0.925

But the parameter estimate is uncertain!!!

```
> print(summary(Fit))

Formula: y ~ 1 - exp(-Theta * x)

Parameters:
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```

Estimated value of the parameter

Standard error of the estimator

$\hat{\theta}$ = 0.0173

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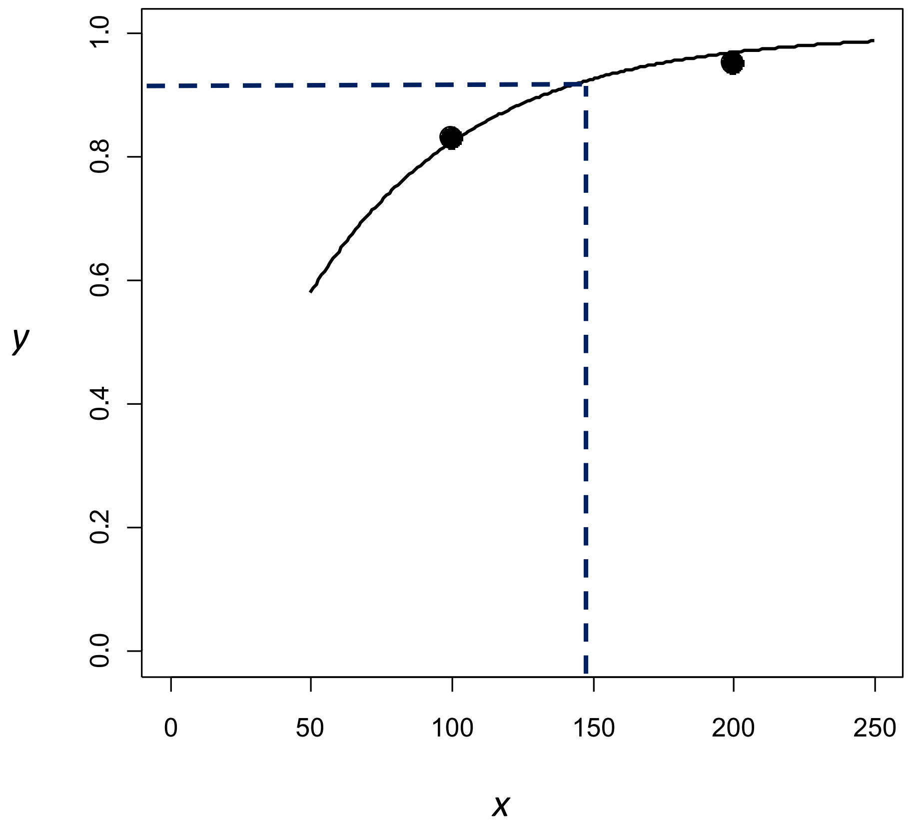


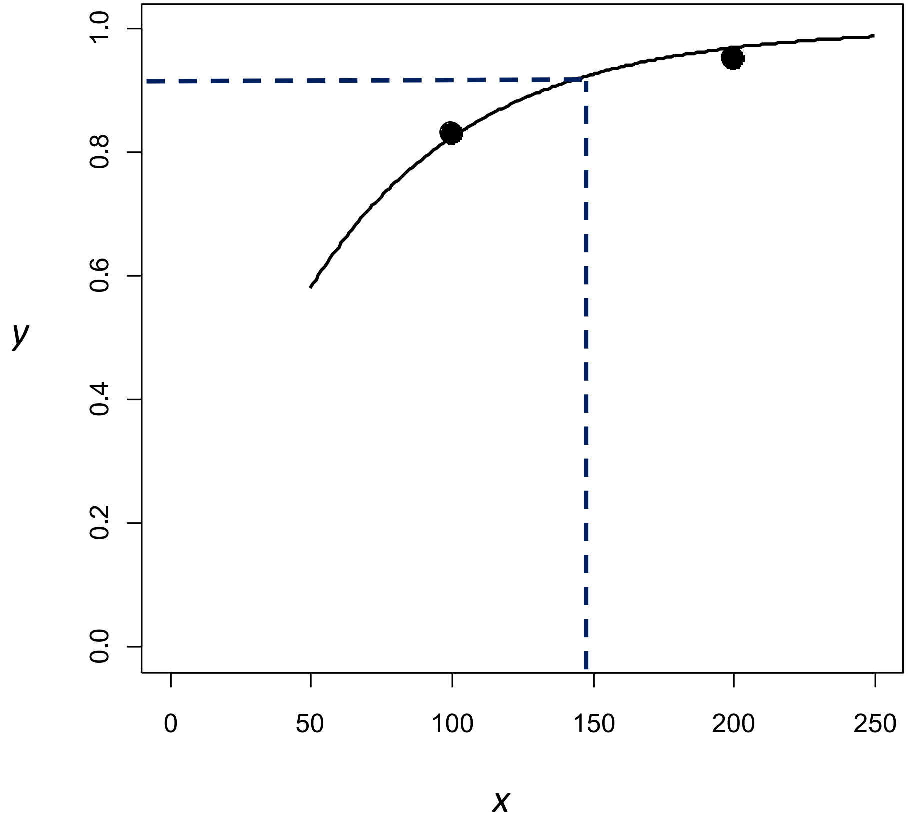
1-exp(-0.0173*150)=0.93

1-exp(-(0.0173+2SE)*150)

1-exp(-(0.0173-2SE)*150)

$\hat{\theta}$ = 0.0173

What is the value of *y* for *x*=150?



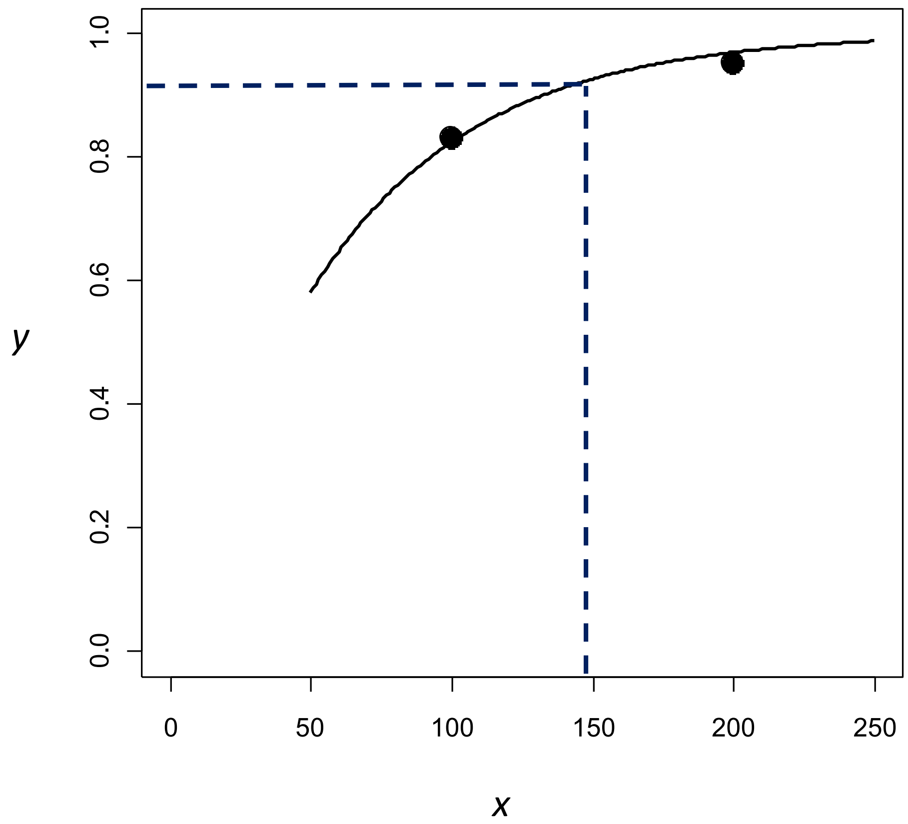
1-exp(-0.0173*150)=0.93

1-exp(-(0.0173+0.002)*150)

1-exp(-(0.0173-0.002)*150)

$\hat{\theta}$ = 0.0173

What is the value of *y* for *x*=150?



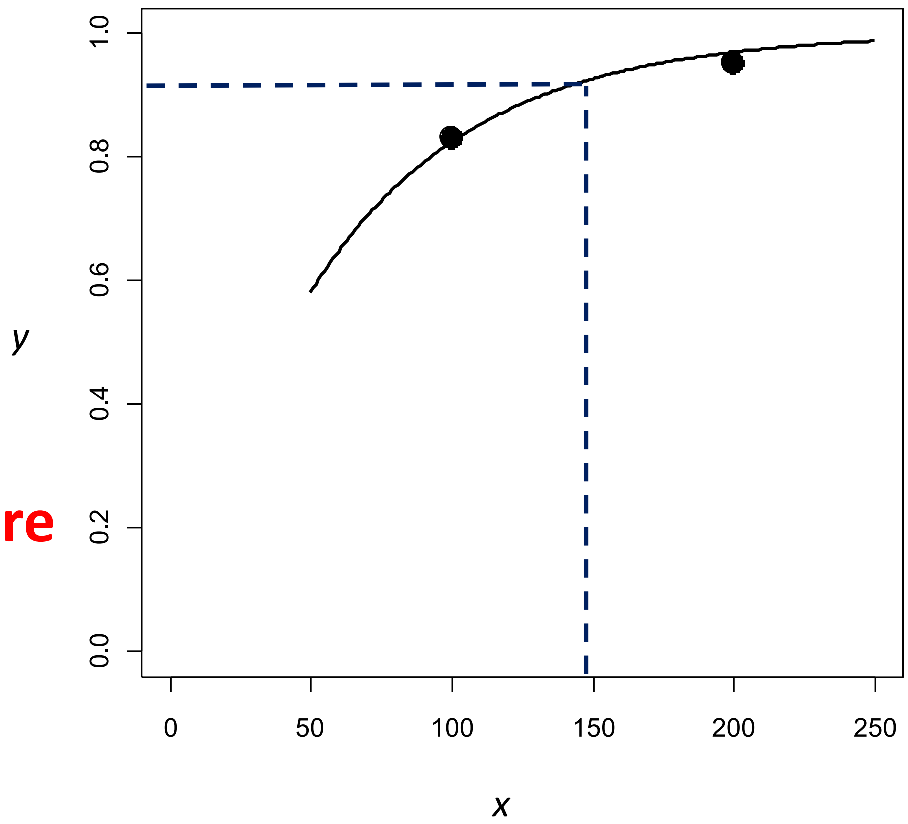
1-exp(-0.0173*150)=0.925

1-exp(-0.0193*150)=0.945

1-exp(-0.0153*150)=0.899

$\hat{\theta} = 0.0173$

What is the value of *y* for *x*=150?



1-exp(-0.0173*150)=0.925

1-exp(-0.0193*150)=0.945

1-exp(-0.0153*150)=0.899

The value is somewhere in the range 0.90-0.95

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