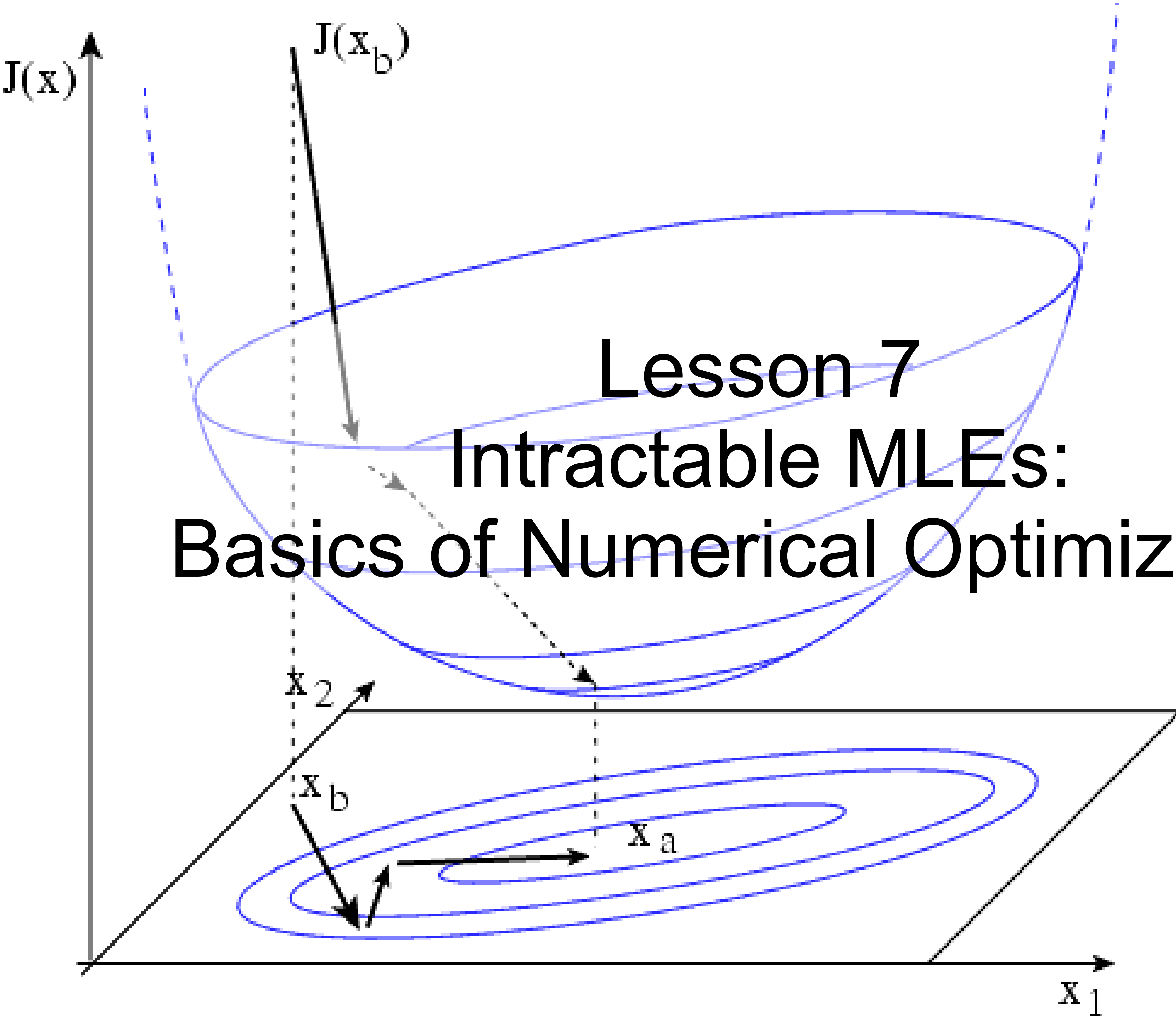
Lesson 7
Intractable MLEs:
Basics of Numerical Optimization



Maximum Likelihood

Write down the Likelihood

Take the log

Take the derivatives w.r.t. each parameter

Set equal to 0 and solve for parameter□□□
Maximum Likelihood Estimate (MLE)

Linear Regression

$$a_0 = \bar{y} - a_1 \bar{x}$$

$$a_1 = \frac{\overline{xy} - \bar{x}\,\bar{y} + a_1 \bar{x}^2}{\overline{x^2}}$$

$$\sigma^2_{ML} = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i \right)^2$$

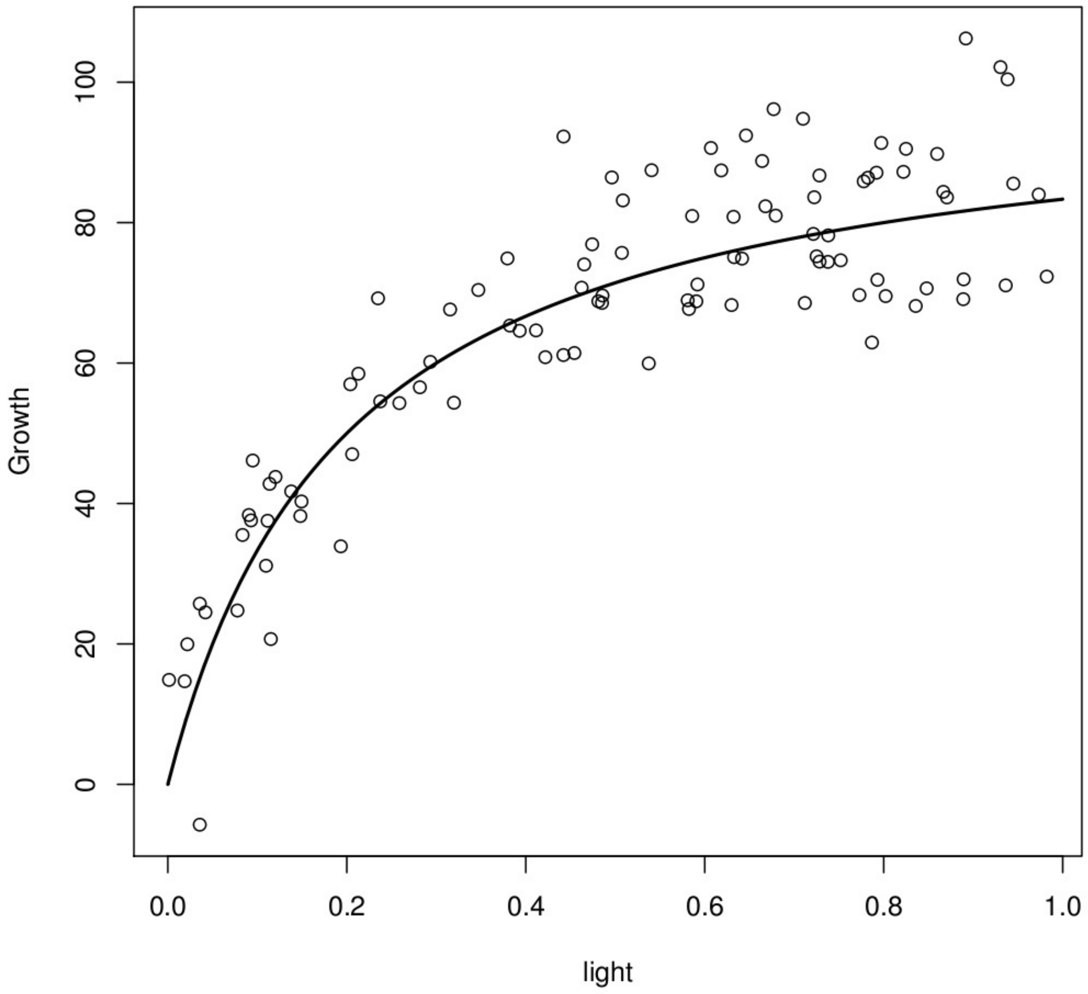
Nonlinear Model Fitting

$$Growth_i = \frac{\beta_1 \, light_i}{\beta_2 + light_i} + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma^2)$$

How do we fit this??

Michaelis-Menten

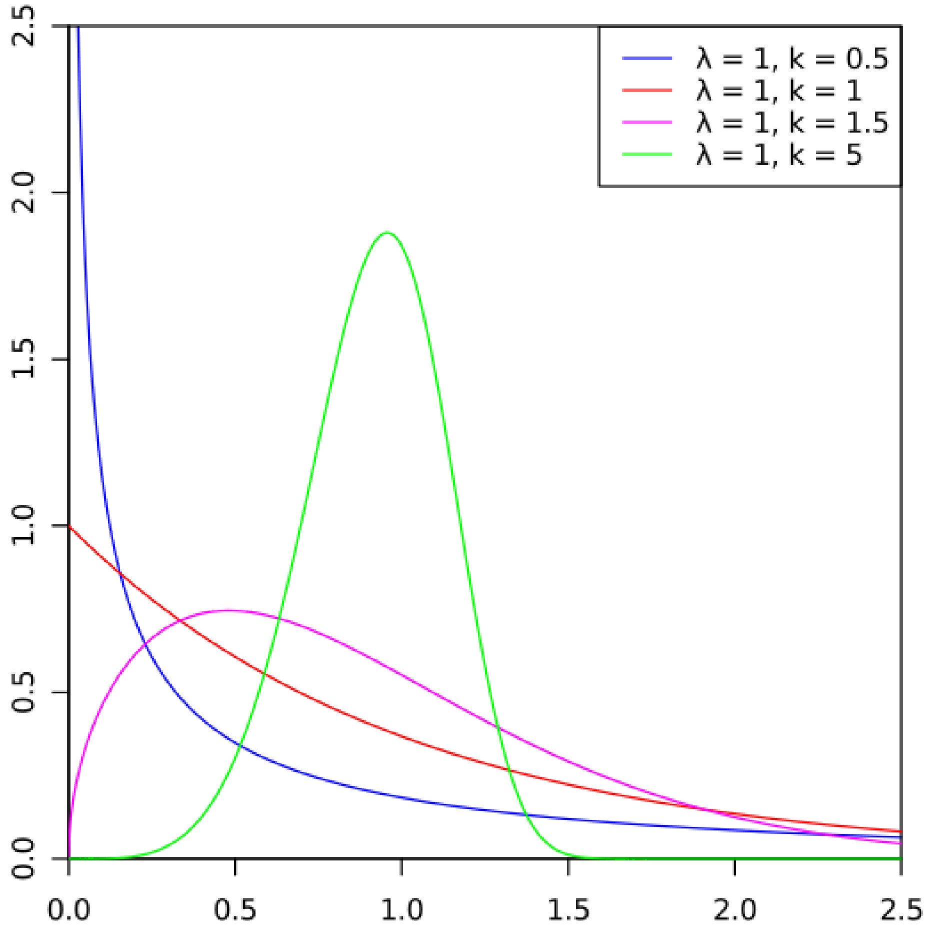


The Problem

- Analytical optimization requires setting the derivative = 0 and solving for the parameter
- For complicated problems a closed-form analytical solution may not exist or may be difficult to solve for.
  - Nonlinear models
  - Multi-parameter models
  - Multiple Constraints

Example – Weibull distribution

$$Weibull(x|c,\lambda) = \left(\frac{c}{\lambda}\right)\left(\frac{x}{\lambda}\right)^{(c-1)} \exp\left(-(x/\lambda)^{c}\right)$$



Example – Weibull distribution

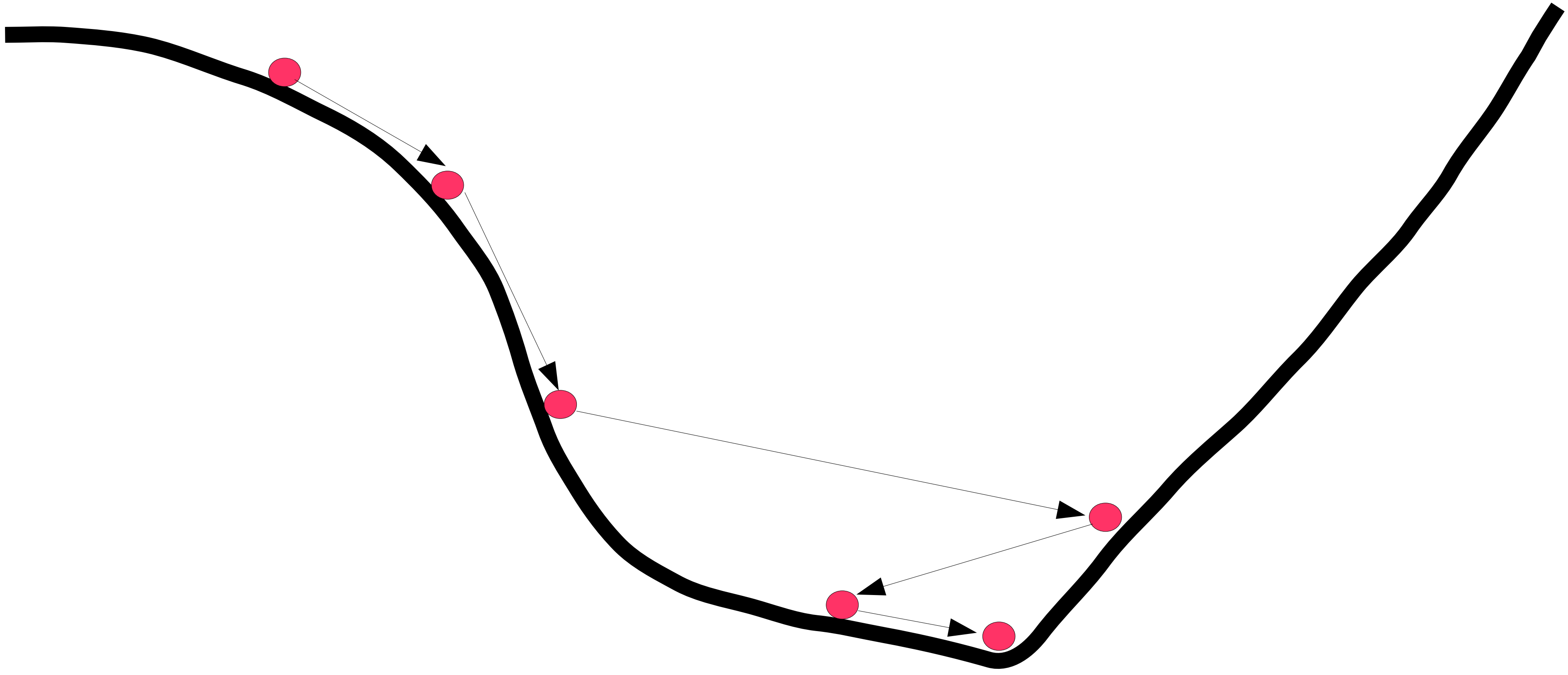
$$Weibull(x|c,\lambda)=\left(\frac{c}{\lambda}\right)\left(\frac{x}{\lambda}\right)^{(c-1)}\exp\left(-(x/\lambda)^{c}\right)$$

$$\ln L=\ln c-\ln\lambda+(c-1)[\ln x-\ln\lambda]-(x/\lambda)^{c}$$

$$\frac{\partial \ln L}{\partial c}=\frac{1}{c}+\ln x-\ln\lambda-\ln c\,(x/\lambda)^{c}=0$$

Not possible to solve for *c* analytically

The Solution:
Numerical Optimization

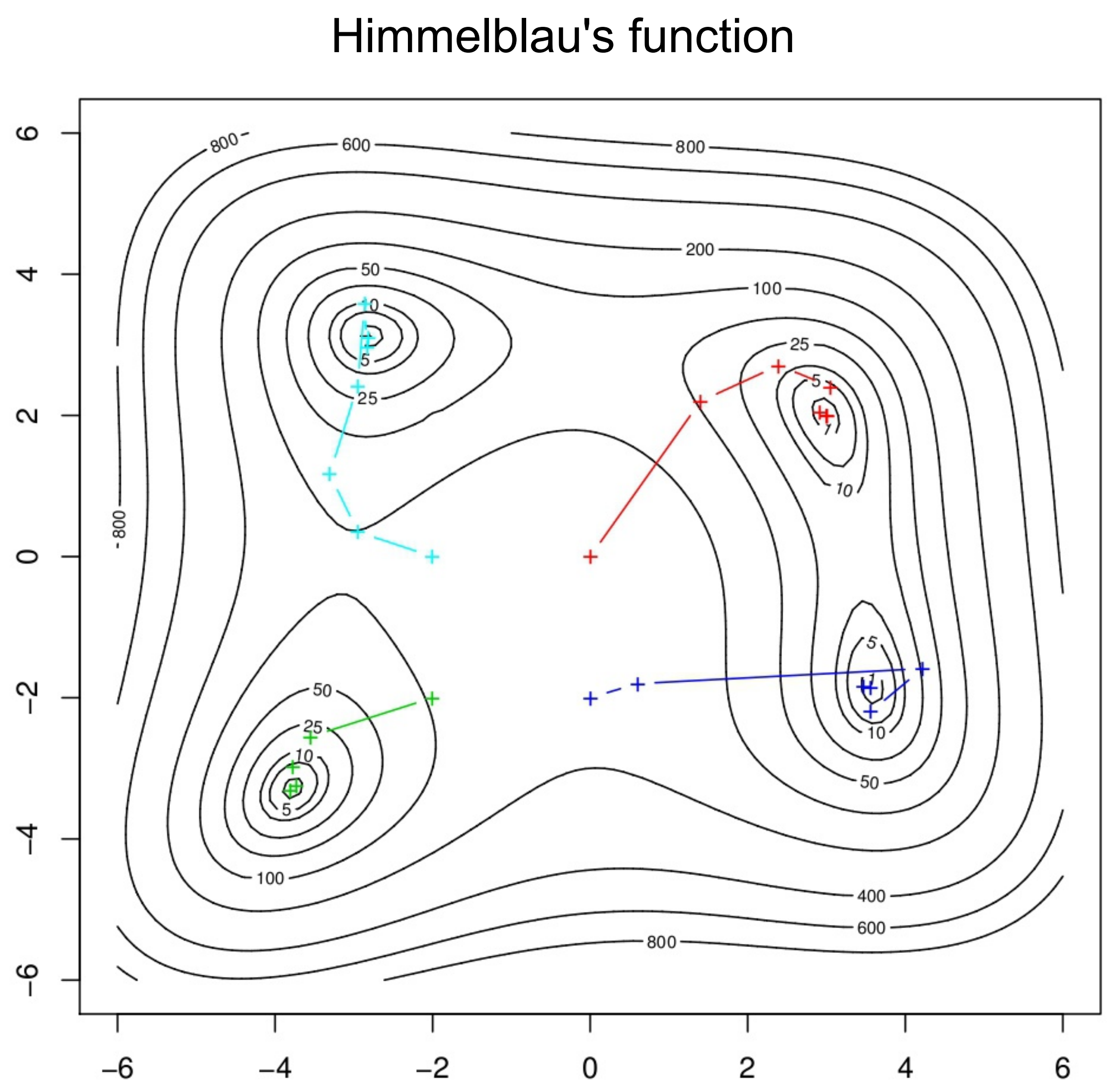


Optimization Algorithm

1) Start from some initial parameter value
2) Evaluate the likelihood
3) Propose a new parameter value
4) Evaluate the new likelihood
5) Decide whether or not to accept the new value
6) Repeat 3-5 until you can't find a better value

1) Start from some initial parameter value

- Far values take a long time to converge
- Can get stuck in local minima
- Want to try multiple initial values



3) Propose a new parameter value

- Diversity of approaches
- Deterministic
  - Gradient decent
  - Nelder-Mead
- Stochastic
  - Genetic algorithms
  - Simulated annealing
- Curvature
  - Newton's method

5) Decide whether or not to accept the new value

- Almost all algorithms accept a new step if it has a lower negative log likelihood
- What if the step has a higher value?
  - Always reject a worse step
    - Efficient
    - More susceptible to local minima
  - Occasionally accept a worse step with some probability
    - Slower convergence
    - Less likely to get caught in local minima

6) Repeat until you can't find a better value

- “Stopping condition”
- Improvement in estimate is below some threshold (gradient)
- Step size is below some threshold
- Failure to converge?
  - Too many steps taken
  - Converged to boundary condition
  - Step size too big (divergence)

Reasons for working with negative log likelihoods

- Log
  - Numerical precision
    - Likelihood is degenerate if a probability = 0
    - In R, taking the log of the returned value is less precise than using “log = TRUE”
- Negative
  - Most numerical optimization routines set up for minimization
- Deviance = -2 log(L)
    - Used in model selection and CI

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Limits to Numerical Methods

- Accuracy
- Generality / Understanding
- Local Minima
- Dimensionality
  - Difficult to explore high dimensional parameter space

MLE Optimization Algorithm

1) Start from some initial parameter value
2) Evaluate the likelihood
3) Propose a new parameter value
4) Evaluate the new likelihood
5) Decide whether or not to accept the new value
6) Repeat 3-5 until you can't find a better value

Simple Example: $y = N(a,\sigma^2)$

Name of the function

Parameter vector

```
lkNormal <- function (beta,y){
  -sum(
    dnorm(y,
          beta[1],
          beta[2],
          log=TRUE)
  )
}
```

Normal density

Response data

a

Standard deviation

Returns the log likelihood

Simple Example: $y = N(a,\sigma^2)$

```
> y = rnorm(10,3.5,2)

> mean(y)
[1] 3.897316

> sd(y)
[1] 2.4483

> lkNormal(c(0,1),y)
[1] 112.1085

> lkNormal(c(3.5,2),y)
[1] 23.06163
```

```
> optim(c(0,1),lkNormal,y=y)
$par
[1] 3.897709 2.323170

$value
[1] 22.61652

$counts
function gradient
      87       NA

$convergence
[1] 0
```

Nonlinear example

$$Growth_i = \frac{\beta_1\, light_i}{\beta_2 + light_i} + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma^2)$$

"Pseudodata"

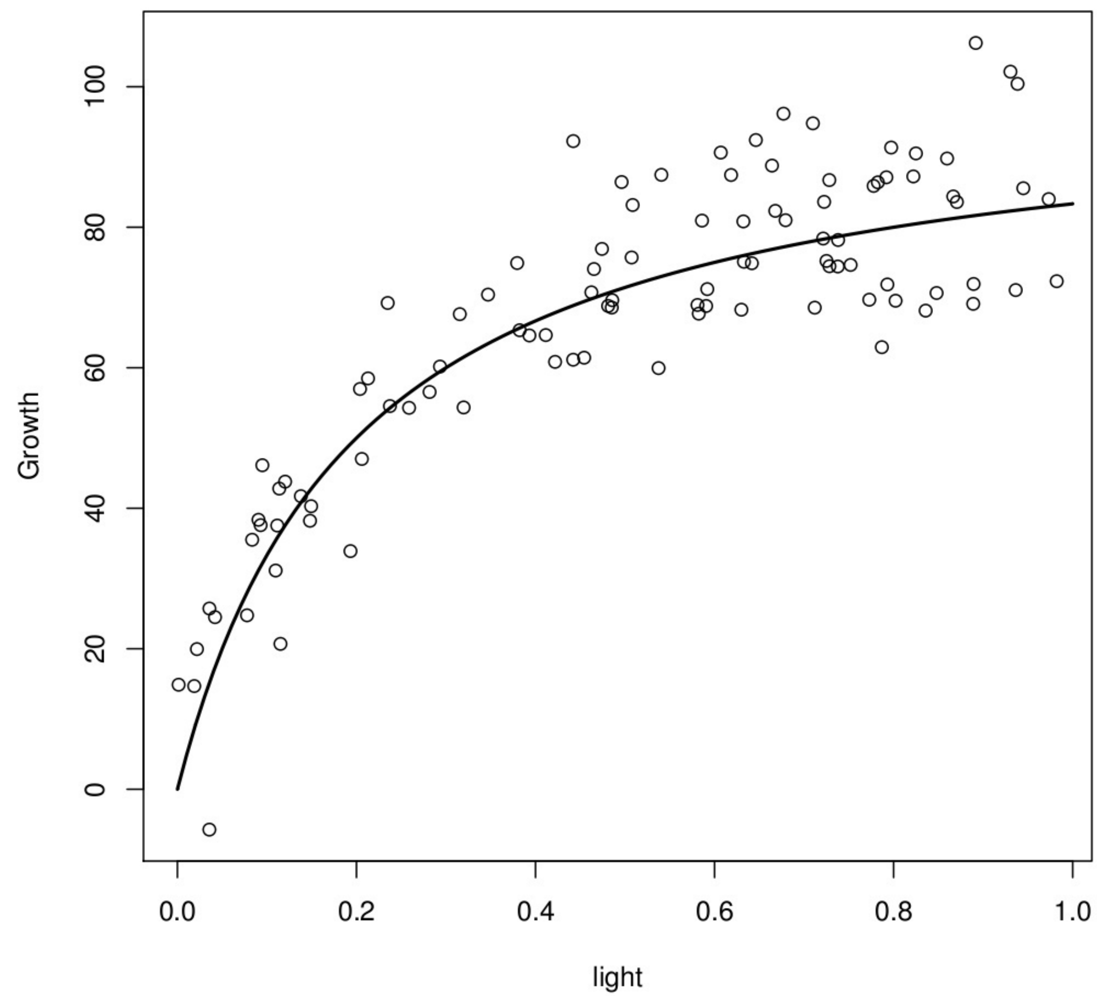
$\cap_1$ = 100

$\cap_2$ = 0.2

σ = 10

n = 100

Michaelis-Menten



Michaelis-Menten negative log likelihood

```
lkMM <- function (beta){
  -sum(
    dnorm(y,
          beta[1]*x/(beta[2]+x),
          beta[3],
          log=TRUE)
  )
}
```

- Name of the function → lkMM
- Parameter vector → (beta)
- Normal density → dnorm
- Response data (growth) → y
- Michaelis-Menten → beta[1]*x/(beta[2]+x)
- Standard deviation → beta[3]
- Returns the log likelihood → log=TRUE

Michaelis-Menten negative log likelihood

```
lkMM <- function (beta){
  -sum(
    dnorm(y,
          beta[1]*x/(beta[2]+x),
          beta[3],
          log=TRUE)
  )
}
```

$$-\sum \log\left(N\left(y \,\middle|\, \frac{\beta_1 x}{\beta_2 + x}, \sigma^2\right)\right)$$

Optimization function

```
opt = optim(
  c(max(y)*0.9,0.5,sd(y)/2),
  lkMM,
  method="L-BFGS-B",
  lower=c(0,0,0),
  upper=c(max(y)*2,1,sd(y)*1.1)
  )
```

Initial conditions → c(max(y)*0.9,0.5,sd(y)/2)

neg log likelihood function → lkMM

Name of algorithm → method="L-BFGS-B"

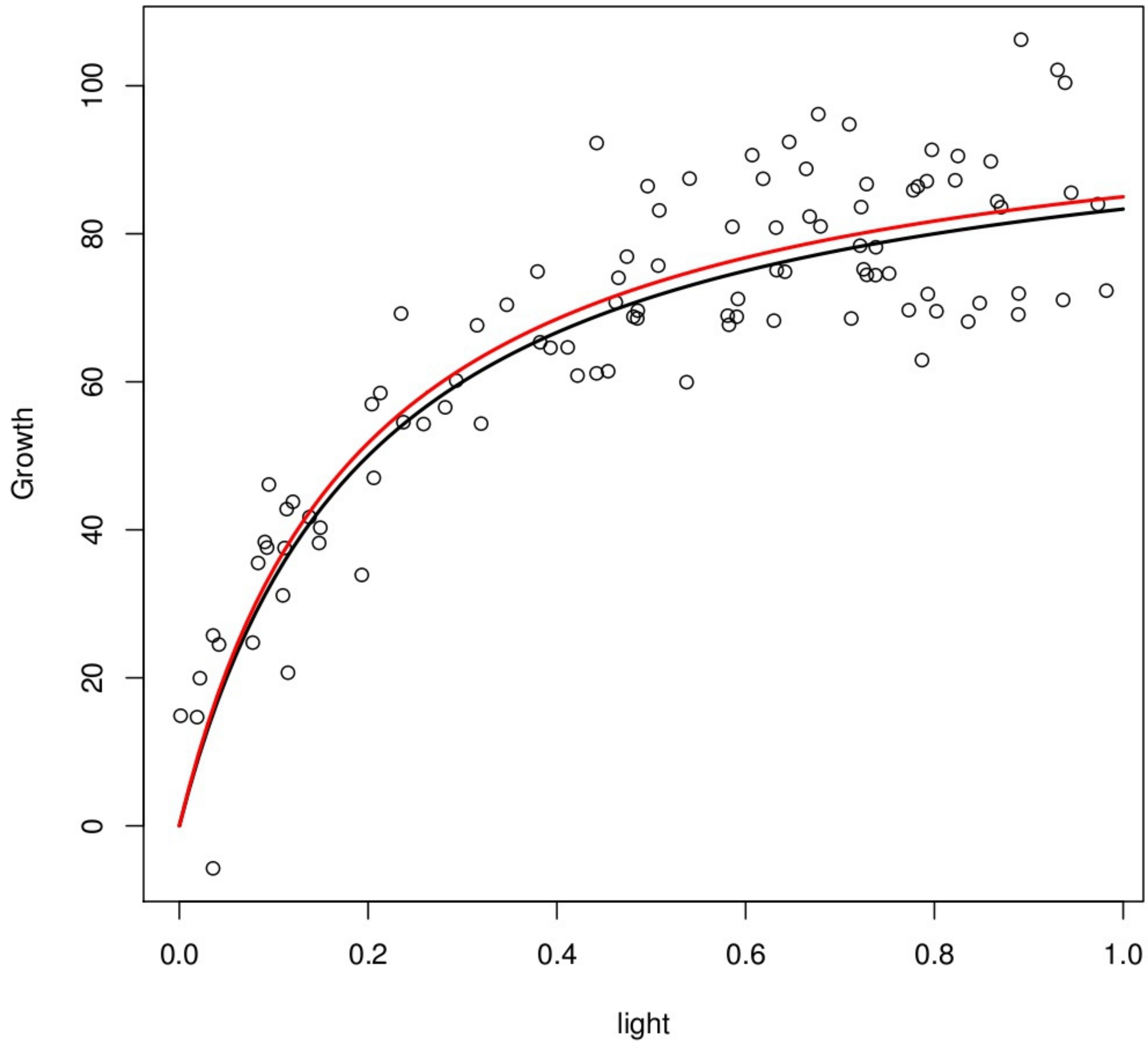
Lower bound → lower=c(0,0,0)

Upper Bound → upper=c(max(y)*2,1,sd(y)*1.1)

Optimization Output

```
> opt
$par
[1] 101.2937369   0.1916526   9.3997657

$value
[1] 365.9635

$counts
function gradient
      48       48

$convergence
[1] 0

$message
[1] "CONVERGENCE: REL_REDUCTION_OF_F <=
FACTR*EPSMCH"
```

“Pseudo”	Fit
$\cap_1$ = 100	101.3
$\cap_2$ = 0.2	0.192
O= 10	9.40
n = 100	



More generally...

- Can fit any 'black box' function
- Can use any distribution
  - No Normality assumption
- Can model the variance explicitly
  - No equal variance assumption
- Various techniques for estimating uncertainties, CI, etc.
- Likelihood is backbone of more advanced approaches (e.g. Bayesian stats)

A few last thoughts on MLE

- More difficult as model complexity increases
- More challenging when not independent
  $P(x1,x2,x3) \neq P(x1)P(x2)P(x3)$
- Require additional assumptions/computation to estimate CI
- Analysis occurs in a “vacuum”
  - No way to update previous analysis