Software tools for Maximum Likelihood Estimation:MB

Lesson 2 - first RTMB & Derivatives

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Jim Bence

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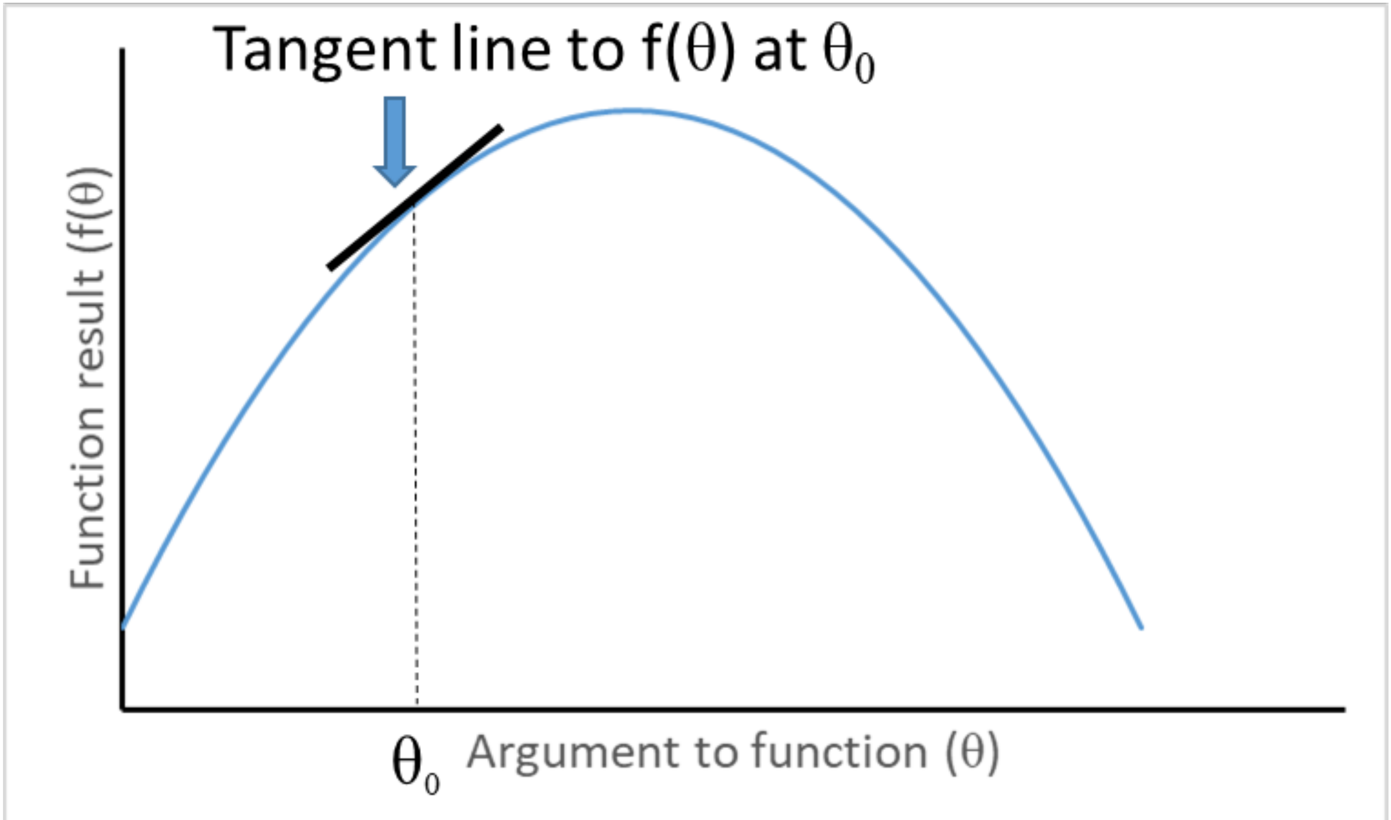
Outline:

- Demos and exercises of using nlminb and RTMB to estimate parameters
- All that derivative stuff
  - Definitions derivatives, partial derivatives, second derivatives, cross derivatives (aka mixed second derivatives), gradient vector and Hessian
- Methods to calculate/appoximate derivatives
- Exercise: finite difference derivatives
- Using the Hessian and gradient vector in parameter searches and to assess uncertainty
- RTMB Nonlinear regression vonb example

Demos of estimating the mean the hard way

- Just using nlminb
- Using RTMB
- Exercise - change model to assume gamma rather than normal (in breakout groups)

What is a derivative



$$\frac{df(\theta)}{d\theta} = \lim h \to 0 \frac{f(\theta + h) - f(\theta)}{h}$$

Partial derivative

Function with multiple arguments but we treat all but one of them as constants, and calculate derivative with respect to just one! E.g.,

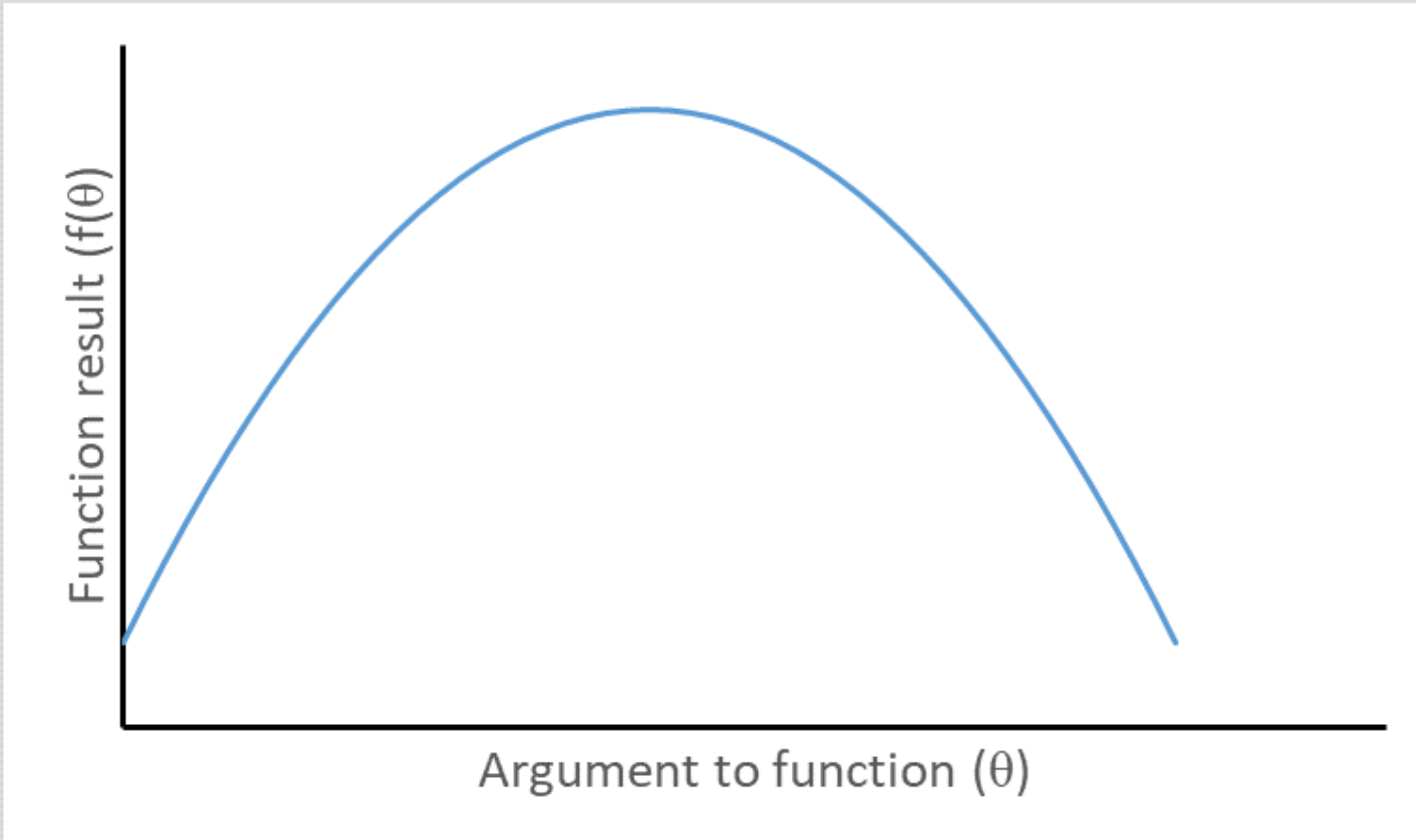
$$\frac{\partial f}{\partial \theta_2} = \lim h \rightarrow 0 \frac{f\left(\theta_1, \theta_2 + h, \theta_3\right) - f\left(\theta_1, \theta_2, \theta_3\right)}{h}$$

Second derivative

Just a derivative of a derivative

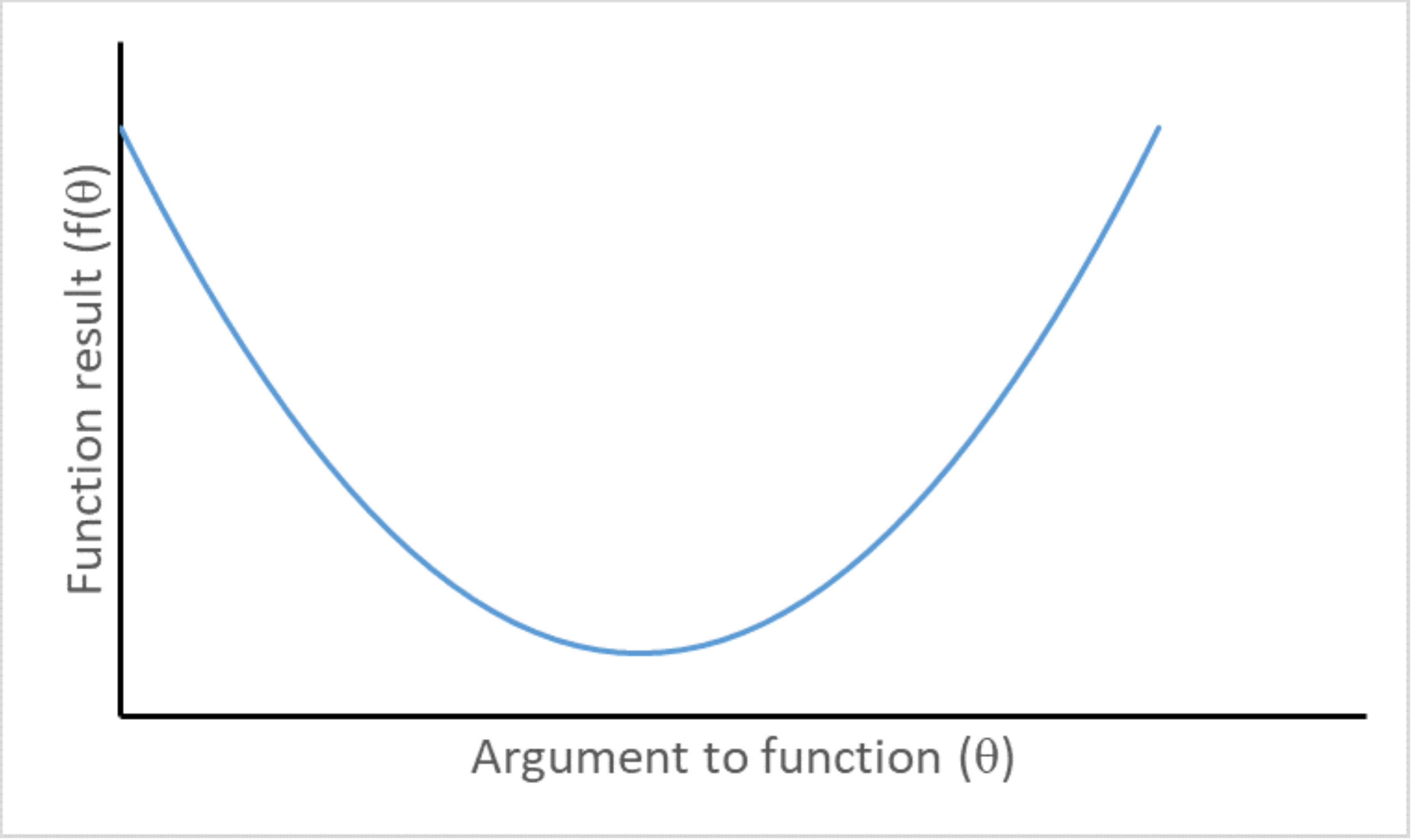
$$\frac{\partial^2 f}{\partial \theta^2} = \frac{\partial \frac{\partial f}{\theta}}{\partial \theta}$$

Visualizing second derivatives



Concave function with negative second derivative

Visualizing second derivatives



Convex function with positive second derivative

Cross derivative (mixed second derivs)

$$\frac{\partial^2 f}{\partial \theta_1 \partial \theta_2} = \frac{\partial \frac{\partial f}{\partial \theta_1}}{\partial \theta_2}$$

An important and convenient fact:

$$\frac{\partial^2 f}{\partial \theta_1 \partial \theta_2} = \frac{\partial^2 f}{\partial \theta_2 \partial \theta_1}$$

Methods for calculating derivatives

- Analytical derivatives. Gold standard but not available for many complex models.
- Finite difference methods. Intuitive but slow and propogate errors.
- Automatic differentiation. Fast and accurate but requires specialized software.

Finite difference derivatives

Widely used, e.g., default of nlminb and Excel solver

Forward difference

$$\partial f / \partial \theta_i = \frac{f\left(\theta_i + h\right) - f\left(\theta_i\right)}{h}$$

h is semi-arbitrary but small relative to θ_i.

Central differences

$$\partial f / \partial \theta_i = \frac{f\left(\theta_i + h\right) - f\left(\theta_i\right)}{h}$$

Exercise - finite difference derivatives

- For g(x) = a + b X + sin X, use finite difference methods to calculate the derivative of g(X) with respect to (wrt) X
  - for x=1, with a=2 and b=0.5. (answer approximately 1.040)
  - Repeat for x=2, a=1, and b=1. Answer approximately 0.5839.
- For a=2, b=0.5, x=1, and same function, use finite differences to find the second derivative wrt x (answer approximately -0.8415)

Automatic differentiation

- Uses repeated applications of chain rule: $\partial z/\partial\theta = [\partial z/\partial y][\partial y/\partial\theta]$
- Simplest case. $y = f(\theta), z = g(y)$, i.e., $z = g(f(\theta))$
- General case we care about:

$$NLL = f_1(f_2(f_3(\ldots f_k(\theta)\ldots)))$$

Gradient

Just a fancy term to mean the vector of derivatives of the NLL function with respect to each parameters (so if k parameters, then k elements)

$$g = \{\partial f/\partial\theta_1, \partial f/\partial\theta_2, \ldots \partial f/\partial\theta_k\}^T$$

Hessian - a square symmetric marix

$$H = \begin{bmatrix} \partial^2 f/\partial\theta_1^2 & \partial^2 f/\partial\theta_1\partial\theta_2 & \dots & \partial^2 f/\partial\theta_1\partial\theta_k \\ \partial^2 f/\partial\theta_2\partial\theta_1 & \partial^2 f/\partial\theta_2^2 & \dots & \partial^2 f/\partial\theta_2\partial\theta_k \\ \dots & \dots & \dots & \dots \\ \partial^2 f/\partial\theta_k\partial\theta_1 & \partial^2 f/\partial\theta_k\partial\theta_2 & \dots & \partial^2 f/\partial\theta_k^2 \end{bmatrix}$$

$$h_{i,j} = h_{j,i} = \frac{\partial^2 f}{\partial\theta_i\partial\theta_j} = \frac{\partial^2 f}{\partial\theta_j\partial\theta_i}$$

If the NLL were a quadratic function as it would be for linear normal model...

$$\theta_{\min} = \theta_{\text{start}} + H^{-1} g$$

where H^{-1} in the matrix inverse of H and $H^{-1} g$ is the product of the inverse of the Hessian and the gradient

Because our models generally not normal and linear, iterative searches...

1. specify starting values for parameters, $\underline{\theta_0}$
2. Replace $\underline{\theta_0}$ by $\underline{\theta_1} = \underline{\theta_0} + \delta_0$
3. Check gradient and Hessian and if at a minimum stop otherwise...
4. Return to step 2 but each time $\underline{\theta_{i+1}} = \underline{\theta_i} + \delta_i$

Newton step: $\underline{\delta}_i = H^{-1}\underline{\mathrm{g}}$ evaluated at current params

Quasi-Newton method uses $\underline{\delta}_i = \lambda H^{-1}\underline{\mathrm{g}}$ with Hessian approximated using search path, and λ a number less than 1

Using the Hessian to calculate asymptotic standard errors

- First some reminders
  - Parameter estimates are random variates that result from estimators (random variables)
  - The variance describes the variability of results from applying the estimation method, namely the expected squared deviation between an estimator and its expected value
  - What we report as a standard error for a parameter is the square-root of this variance.

The variance-covariance matrix

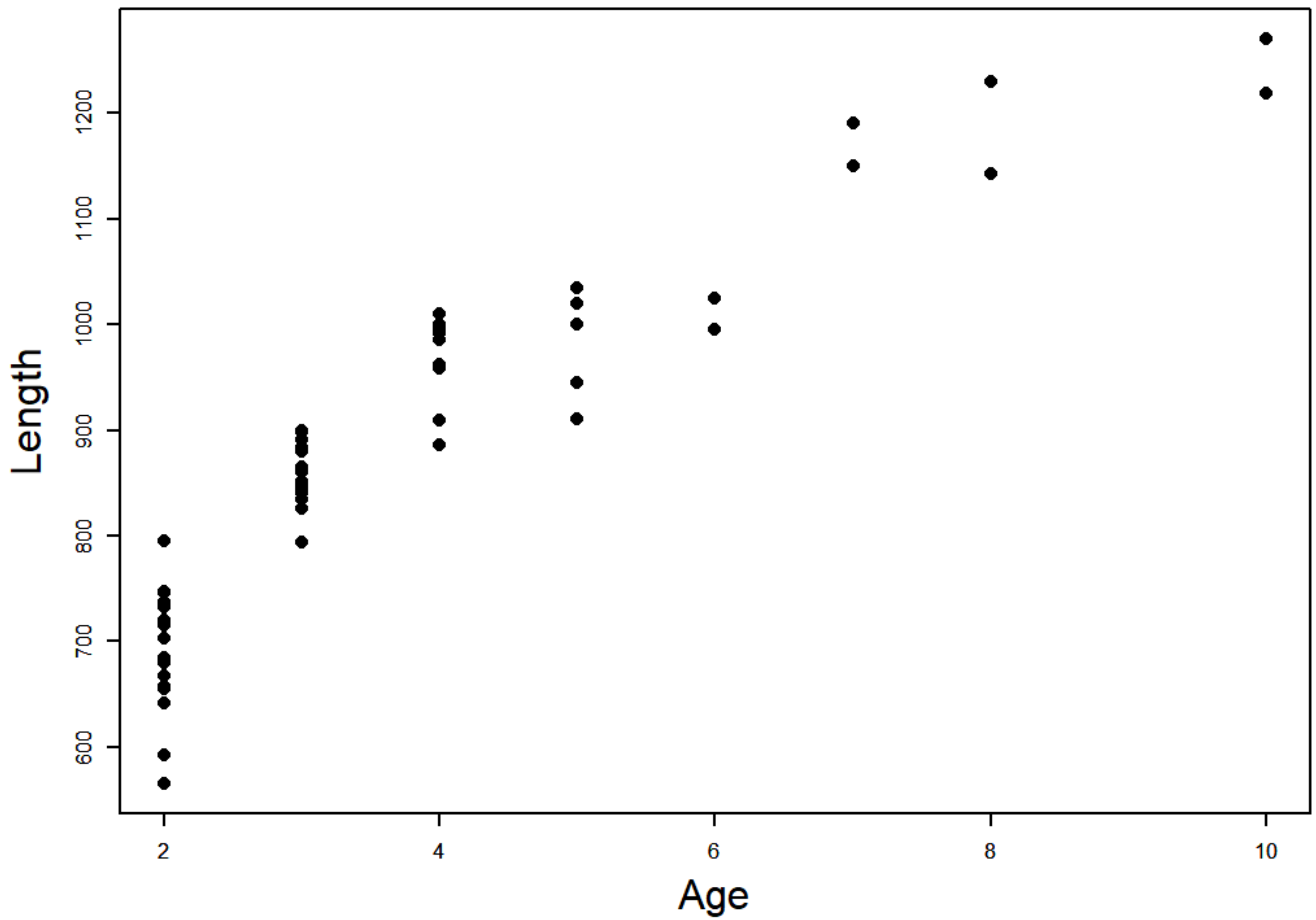
$$\Sigma = \begin{matrix} \sigma_1^2 & \sigma_{1,2} & \ldots & \sigma_{1,k} \\ \sigma_{2,1} & \sigma_2^2 & \ldots & \sigma_{2,k} \\ \ldots & \ldots & \ldots & \ldots \\ \sigma_{k,1} & \sigma_{k,2} & \ldots & \sigma_k^2 \end{matrix}$$

The asymptotic variance-covariance matrix

$$\hat{\Sigma} = H^{-1}$$

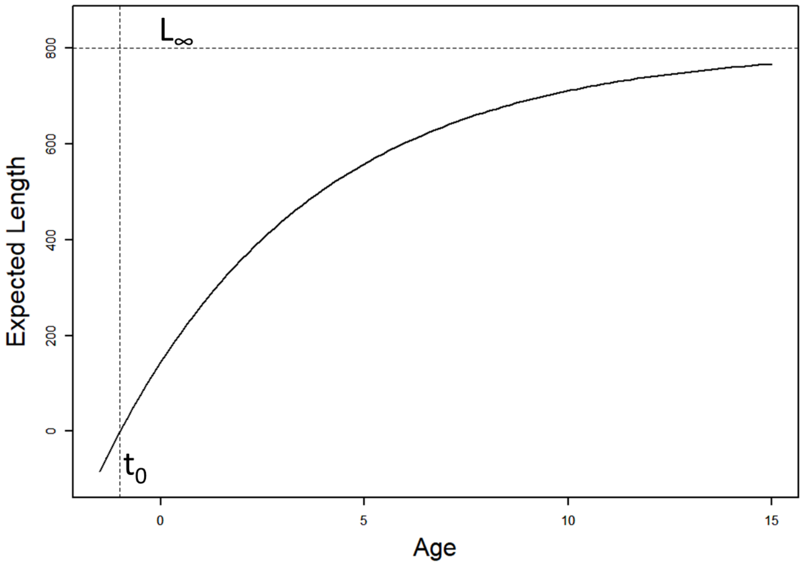
- Square-root of diagonal gives standard errors
- Off-diagonals are covariances
- The Hessian needs to be positive definite for the calculation
- If the Hessian is not positive definite its a problem!
- Delta method used to obtain SEs for derived quantities (using $\hat{\Sigma}$)

Musky vonB example



musky_vonb.dat

von Bertalanffy model

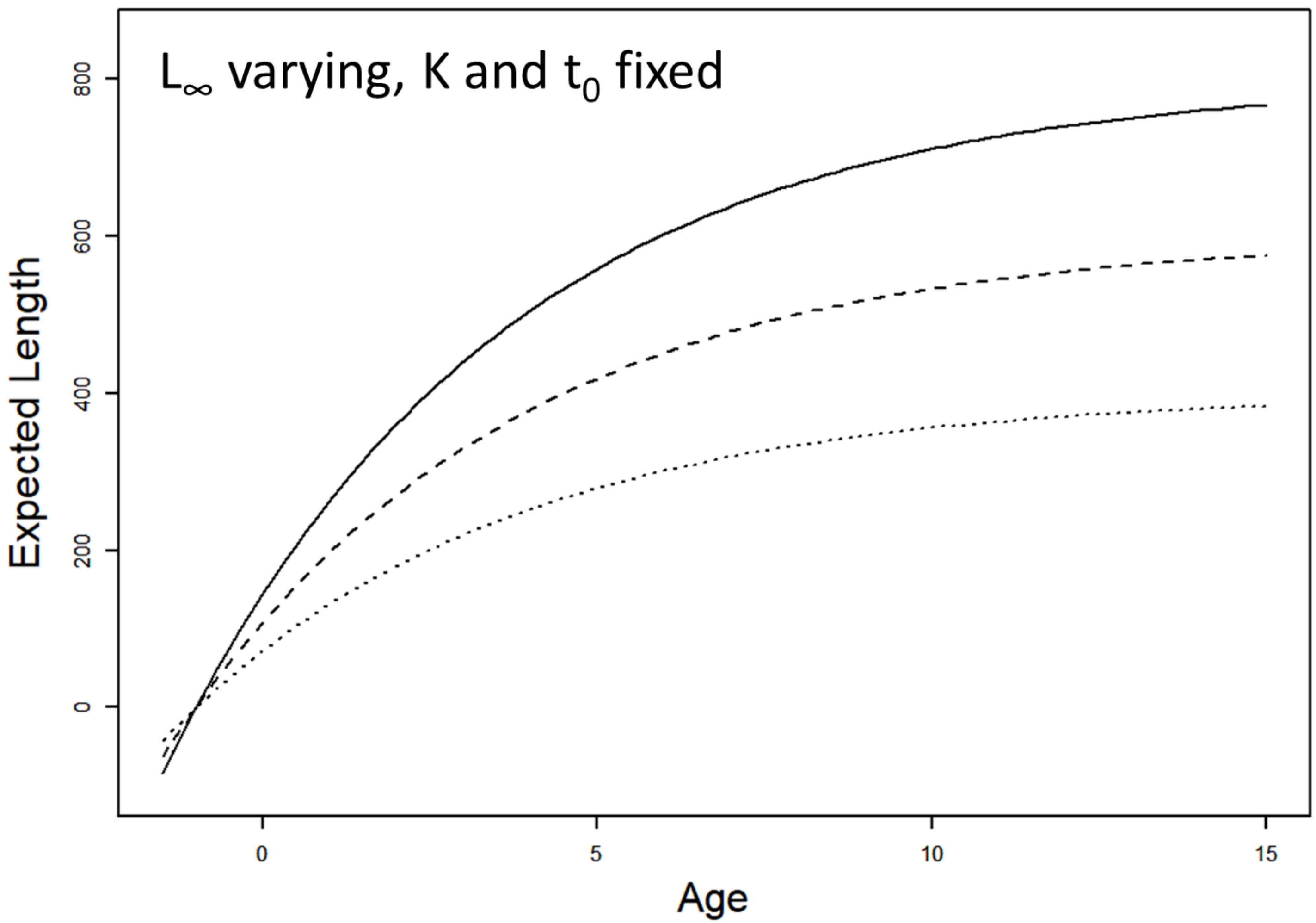


$$L_i = L_\infty \left(1 - e^{-K(a_i - t_0)}\right) + \varepsilon_i$$

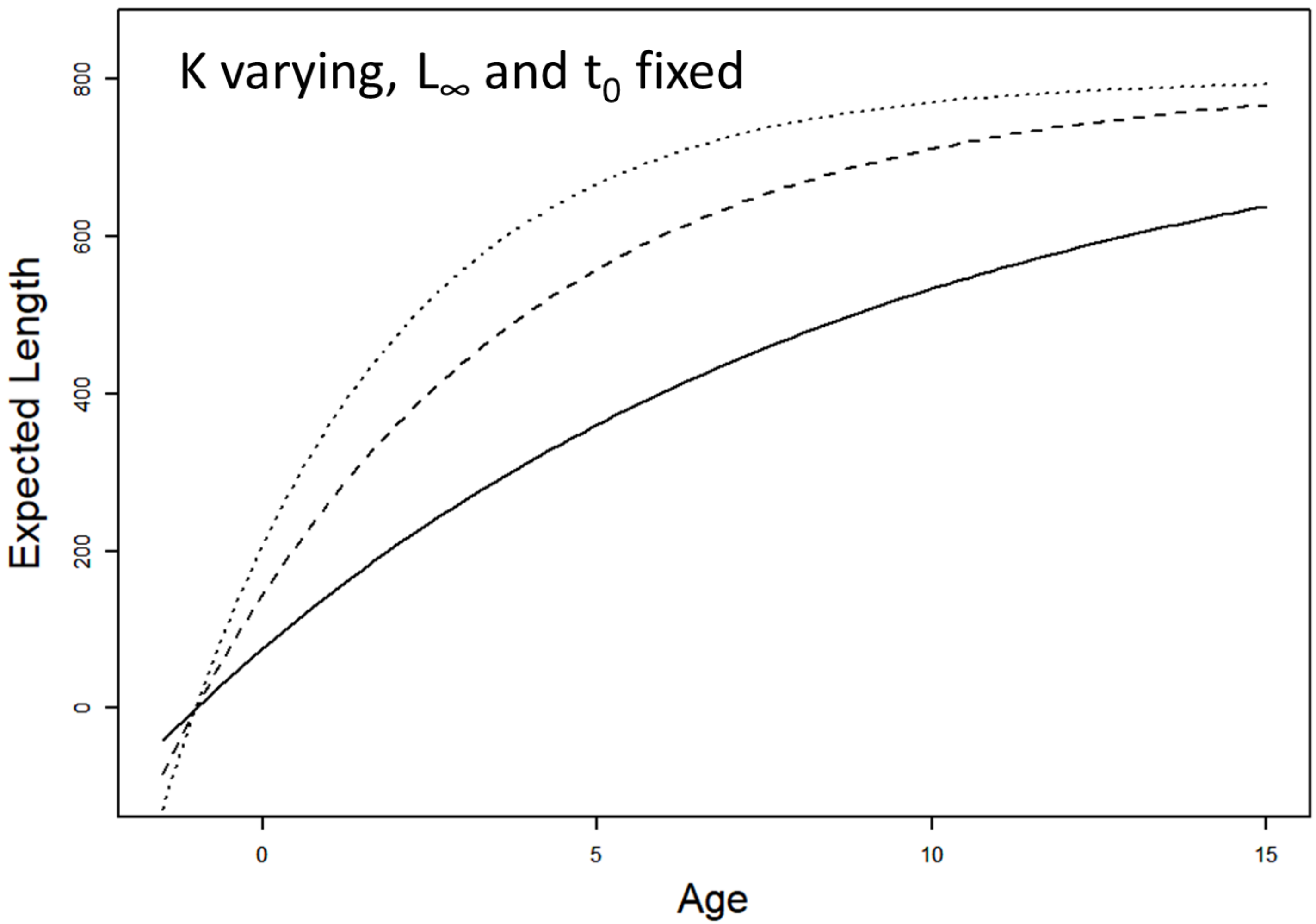
$$\varepsilon_i \overset{iid}{\sim} N\left(0, \sigma^2\right)$$

$$L_i \sim N\left(L_{a_i}, \sigma^2\right)$$

Influence of Linf



Influence of K



Musky vonB setup code

```
library(RTMB);

gmRdat = read.table("lesson2/data/musky_vonb.dat",head=T);

#Set up the data and starting value of parameters for RTMB
gmdat = list(len_obs=gmRdat[,"Length"],age=gmRdat[,"Age"]);
gmpar = list(log_linf=7,log_vbk=-1.6,t0=0,log_sd=4);
```

code for NLL for Musky vonb example

```
NLL_fun = function(par_lst){
  getAll(gmdat,par_lst);
  linf = exp(log_linf);
  vbk = exp(log_vbk);
  sd = exp(log_sd);
  len_pred = linf * (1 - exp(-vbk * (age - t0)));
  nll = -sum(dnorm(len_obs, len_pred, sd, TRUE));
  atage_pred = linf * (1 - exp(-vbk * ((1:11) - t0)))
  REPORT(atage_pred);
  nll
}
```

Create model object and print predicted lengths before fitting model

```
obj <- MakeADFun(NLL_fun,gmpar);

GMreport=obj$report();
GMreport
```

```
$atage_pred
 [1] 200.4870 364.3209 498.2026 607.6080 697.0118 770.0708 829.7731 878.5606
 [9] 918.4287 951.0082 977.6314
```

fit the model

```
fit = nlminb(obj$par, obj$fn, obj$gr);
```

```
outer mgc:  3572.344
outer mgc:  115.0372
outer mgc:  306.8376
outer mgc:  101.0471
outer mgc:  30.69436
outer mgc:  135.1418
outer mgc:  120.5931
outer mgc:  25.99566
outer mgc:  197.1401
outer mgc:  122.5854
outer mgc:  66.52428
outer mgc:  36.54847
outer mgc:  3.778352
outer mgc:  19.59957
outer mgc:  1.539833
```

Get parameter uncertainties and convergence diagnostics

```r
sdr = sdreport(obj);
```

```
outer mgc:  0.0001970265
outer mgc:  19.77567
outer mgc:  19.71682
outer mgc:  9.178336
outer mgc:  9.171702
outer mgc:  2.35869
outer mgc:  2.358392
outer mgc:  0.1198859
outer mgc:  0.1201142
```

```r
sdr #summary(sdr)
```

```
sdreport(.) result
           Estimate Std. Error
log_linf  7.1488714 0.04083255
log_vbk  -1.2456407 0.16950408
t0       -0.7710237 0.35092437
log_sd    3.8876390 0.09128707
Maximum gradient component: 0.0001970265
```

Predicted lengths at age after model fitting

```
GMreport = obj$report();
GMreport;
```

```
$atage_pred
 [1]  508.1491  699.3217  842.6904  950.2090 1030.8420 1091.3122 1136.6614
 [8] 1170.6709 1196.1760 1215.3035 1229.6480
```

vonB Exercises

- Change REPORT(atage_pred) to ADREPORT(atage_pred) and look at sdreport and summary of the sdreport
- Calculate a new variable equal to vbk*linf as ADREPORT
- Change the model so data are assumed gamma distributed (with expected value given by vonB equation and constant variance)