Introduction to nonlinear parameter estimation, likelihoods and AD Model Builder

ADMB Short Course
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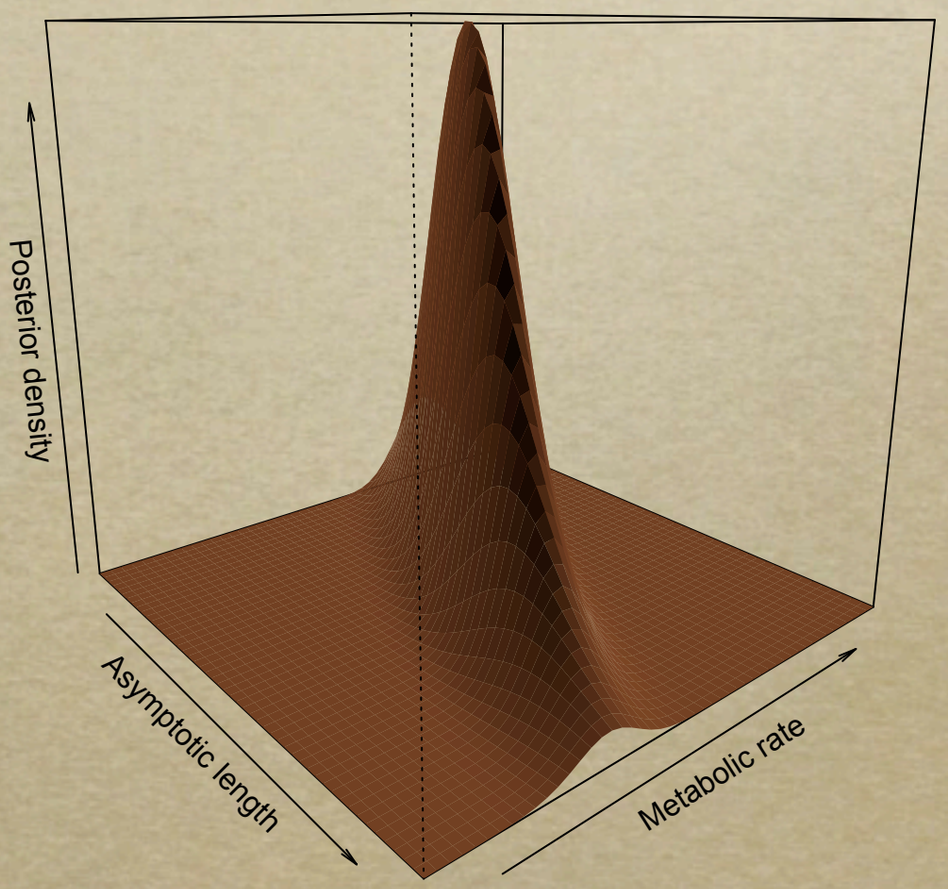
Optimization methods

- *Brute Force (Grid based)*
- *Derivative-based methods*
  - *e.g., Newtons' method*
- *derivative free methods*
  - *simplex method*



Derivative based methods

- *Most algorithms use finite differences*

$$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x} \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

- *i.e. a numerical approximation to the derivative; Simple, Inaccurate, & Slow.*

Analytical Derivatives

- *ADMB uses analytical derivatives;*
  less simple, more accurate, & fast
  - *ADMB carries out the not-so simple derivative calculations behind the scenes!*

Numerical vs Analytical derivatives

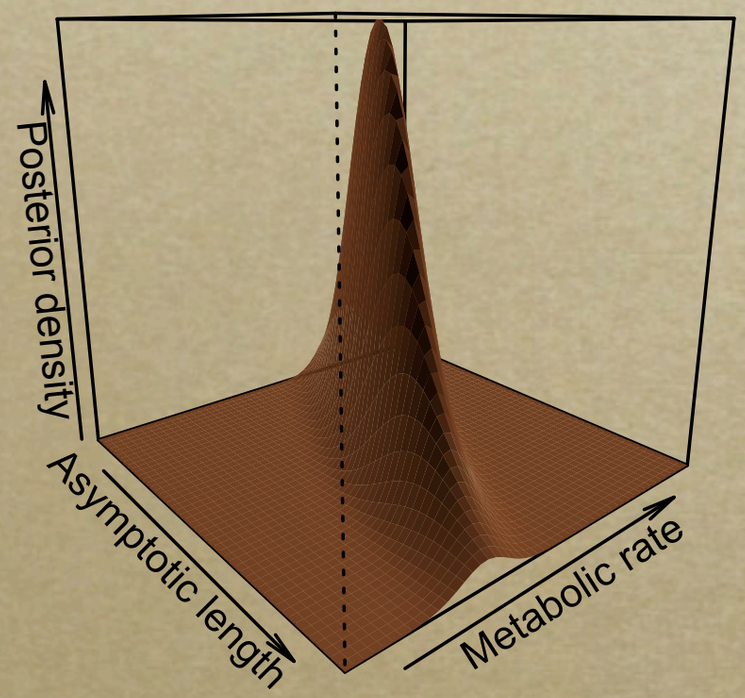
$$f(x) = 5x - \ln(x); \quad f'(x) = 5 - 1/x; \quad f''(x) = 1/x^2$$

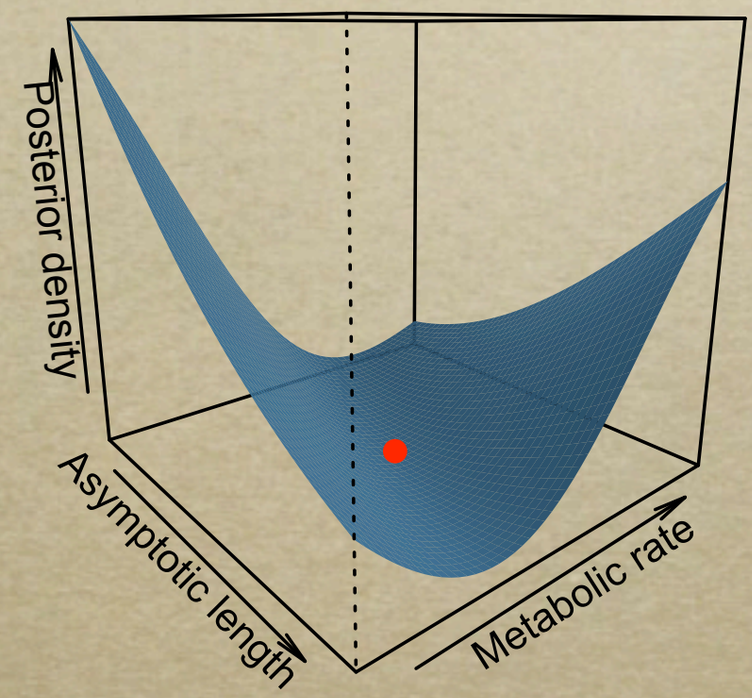
	Analytical Derivative			Numerical derivative		
Iteration	x	f'(x)	f''(x)	x	f'(x)	f''(x)
1	0.01	-9.5E+01	1E+04	0.01	-9.45E+01	9.8E+03
2	0.0195	-4.63E+01	2.63E+03	0.01964	-4.58E+01	2.57E+03
3	0.0371	-2.2E+01	7.27E+02	0.03748	-2.16E+01	7.08E+02
4	0.0673	-9.86E+00	2.21E+02	0.06805	-9.68E+00	2.15E+02
5	0.112	-3.93E+00	7.98E+01	0.11303	-3.84E+00	7.81E+01
6	0.1613	-1.2E+00	3.85E+01	0.16222	-1.16E+00	3.8E+01
7	0.1925	-1.95E-01	2.7E+01	0.19285	-1.84E-01	2.69E+01
8	0.1997	-7.1E-03	2.51E+01	0.1997	-6.22E-03	2.5E+01
9	0.2	0E+00	2.5E+01	0.19995	-4.61E-06	2.5E+01
10	0.2	0E+00	2.5E+01	0.19995	2E-09	2.5E+01
11	0.2	0E+00	2.5E+01	0.19995	0E+00	2.5E+01

Minimize negative log-likelihood

$$L(y_i|\mu,\sigma) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y_i-\mu)^2}{2\sigma^2}\right]$$

$$\ell(y_i|\mu,\sigma) = n\left[\ln(\sigma) + \frac{1}{2}\ln(2\pi)\right] + \sum_{i=1}^{n} \frac{(y_i-\mu)^2}{2\sigma^2}$$





Likelihoods

$$\ell(data|\Theta)$$

What is a likelihood

- *A likelihood function is a probability model.*

$$\ell(data|\Theta)$$

- *What is the likelihood of the data given the parameters?*
- *We treat the data as fixed and vary the parameters to find the most likely values*

Why do we use -ve log likelihoods?

- *Likelihoods are multiplicative*

$$L(y_i|\mu,\sigma) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y_i-\mu)^2}{2\sigma^2}\right]$$

- *log likelihoods are additive*

$$\ell(y_i|\mu,\sigma) = n\left[\ln(\sigma) + \frac{1}{2}\ln(2\pi)\right] + \sum_{i=1}^{n} \frac{(y_i-\mu)^2}{2\sigma^2}$$

- *what happens if the number of observations gets very large?*

Four common negative log likelihoods kernels

Normal $$\ell(x_i|\mu,\sigma) = n\ln(\sigma) + \frac{\sum_i (x_i-\mu)^2}{2\sigma^2}$$

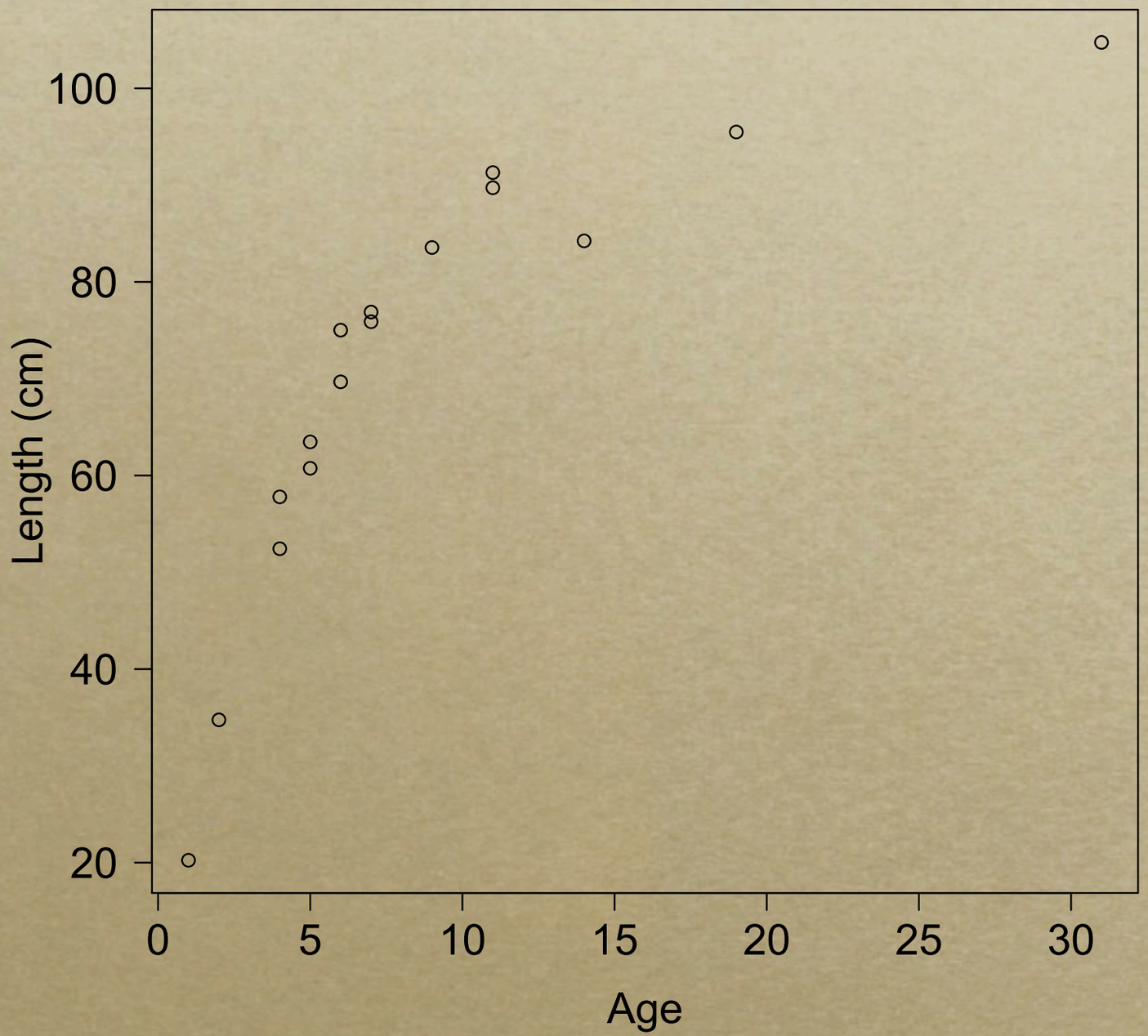
Lognormal $$\ell(x_i|\mu,\sigma) = n\ln(\sigma) + \sum_i \ln(x_i) + \frac{\sum_i (\ln(x_i)-\mu)^2}{2\sigma^2}$$

Poisson $$\ell(x_i|\mu_i) = \sum_i \mu_i \ln(x_i) - \sum_i \mu_i$$

Multinomial $$\ell(x_i|p_i) = \sum_i x_i \ln(p_i)$$

Example
- a simple growth model

Exercise: von Bertalanffy growth



age	length
9	84
11	90
11	91
7	77
6	70
7	76
5	63
4	58
6	75
2	35
1	20
5	61
4	52
19	95
31	105
14	84

ADMB Template -Bare Bones-

- DATA_SECTION
  - read in data and process data using LOC_CALCS
- PARAMETER_SECTION
  - declare model parameters
  - objective_function_value f; //minimize this value
  - declare global dvariables
- PROCEDURE_SECTION
  - define model procedures and calculate f;
  - must use “;” at the end of each line
- REPORT_SECTION
  - write results to a report file.

Model notation

Data

$$a_i, l_i$$

Parameters

$$l_\infty, k$$

Model & Residuals

$$\hat{l}_i = l_\infty \left(1 - \exp(-ka)\right) + \epsilon_i$$

$$\epsilon_i = l_i - \hat{l}_i$$

$$\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \epsilon_i^2}$$

Negative loglikelihood

$$\ell(l_i | l_\infty, k, \tau) = n\left[\ln(\sigma) + \tfrac{1}{2}\ln(2\pi)\right] + \sum_{i=1}^{n} \frac{\epsilon_i^2}{2\sigma^2}$$

How ADMB works

- A 3 step process:
  - tpl2cpp.exe -- translates the *.tpl to a *.cpp file
  - adcomp -- translates the *.cpp file to *.obj file
    - adlink -- links the *.obj file to an *.exe file
- Errors can occur at each of these steps; this is useful for tracking down coding errors.
- Always use the -s option when developing models (safe model with array bound checking).

The data file

- default file name is the program name with the extension .dat

vonB.dat — untitled

vonBdem.R | vonB.dat | NewtonMethod.R

```
#nobs
16
#age    length
9   84
11  90
11  91
7   77
6   70
7   76
5   63
4   58
6   75
2   35
1   20
5   61
4   52
19  95
31  105
14  84
```

Line: 16 Column: 1 Plain Text Tab Size: 4

ADMB Template file

- use init_ prefix to read data from file

vonB.tpl — untitled

vonBdem.R | vonB.dat | vonB.tpl | NewtonMethod.R

```
1  DATA_SECTION
2      init_int nobs;
3      init_matrix data(1,nobs,1,2);
4      vector a(1,nobs);
5      vector l(1,nobs);
6      LOC_CALCS
7        a=column(data,1);
8        l=column(data,2);
9      END_CALCS
10 PARAMETER_SECTION
11
12 PROCEDURE_SECTION
13
14 REPORT_SECTION
15
16
```

Line: 10 Column: 18 ADMB Tab Size: 4

ADMB Template file

- Use init_ prefix to declare parameters & !! is shorthand for LOC_CALCS

vonB.tpl — untitled

vonBdem.R | vonB.dat | vonB.tpl | NewtonMethod.R

```
    init_int nobs;
    init_matrix data(1,nobs,1,2);
    vector a(1,nobs);
    vector l(1,nobs);
    LOC_CALCS
      a=column(data,1);
      l=column(data,2);
    END_CALCS

PARAMETER_SECTION
    init_number linf; //asymptotic length
    init_number k;     //metabolic rate parameter
    !! linf=max(l);  //initial value for linf
    !! k=0.2;        //initial guess for k
    objective_function_value f;
    vector lhat(1,nobs);

PROCEDURE_SECTION

REPORT_SECTION
```

Line: 17 Column: 25 ADMB Tab Size: 4 lhat

ADMB Template

- Calculate objective function in the PROCEDURE SECTION

vonB.tpl — untitled

vonBdem.R | vonB.dat | vonB.tpl | NewtonMethod.R

```
    DATA_SECTION
      a=column(data,1);
      l=column(data,2);
    END_CALCS

PARAMETER_SECTION
    init_number linf; //asymptotic length
    init_number k;     //metabolic rate parameter
    !! linf=max(l);  //initial value for linf
    !! k=0.2;        //initial guess for k
    objective_function_value f;
    vector lhat(1,nobs);

PROCEDURE_SECTION
    lhat=linf*(1.-exp(-k*a));
    dvar_vector epsilon=l-lhat; //local declaration
    dvariable sigma=sqrt(var(epsilon));
    f=nobs*(log(sigma)+0.5*log(2.*3.141593))
      +sum(square(epsilon))/(2.*sigma*sigma);

REPORT_SECTION
```

Line: 25 Column: 1 ADMB Tab Size: 4 log

ADMB Vs. optim() in R

ADMB (n=12 function evaluations, f=42.680)

Parameter	MLE	SD	Correlation linf	k
linf	99.000	2.210	1.00	
k	0.207	0.012	-0.85	1.00

R (n=29 function evaluations, f=42.695)

Parameter	MLE	SD	Correlation linf	k
linf	99.000	2.216	1.00	
k	0.207	0.012	-0.84	1.00

Tools for estimating uncertainty in ADMB

Methods for estimating uncertainty

- Inverse Hessian
- Profile likelihood
- Markov Chain Monte Carlo (MCMC)

Inverse Hessian

- ADMB uses the delta method to calculate the inverse hessian.

$$H = \frac{\partial^2 \ell}{\partial \Theta_i \partial \Theta_j}$$

- H^{-1} approximates the covariance matrix if the objective function is quadratic near its minimum.
- Standard deviations for all parameters, sdreport and likprof variables

vonb.std — ADMB Course

vonB.tpl | vonb.rep | vonb.prf | vonb.par | vonb.std | vonBdem.R

```
index   name      value       std dev
    1   linf      9.9007e+01 2.2078e+00
    2   k         2.0701e-01 1.1987e-02
    3   lp_linf   9.9007e+01 2.2078e+00
    4   std_len   1.8513e+01 6.5120e-01
    5   std_len   3.3565e+01 1.0124e+00
    6   std_len   4.5802e+01 1.1751e+00
    7   std_len   5.5750e+01 1.2094e+00
    8   std_len   6.3839e+01 1.1692e+00
    9   std_len   7.0415e+01 1.0971e+00
   10   std_len   7.5761e+01 1.0273e+00
   11   std_len   8.0108e+01 9.8511e-01
   12   std_len   8.3642e+01 9.8446e-01
   13   std_len   8.6515e+01 1.0256e+00
   14   std_len   8.8851e+01 1.0987e+00
   15   std_len   9.0750e+01 1.1911e+00
   16   std_len   9.2294e+01 1.2919e+00
   17   std_len   9.3550e+01 1.3934e+00
   18   std_len   9.4570e+01 1.4909e+00
   19   std_len   9.5400e+01 1.5816e+00
   20   std_len   9.6074e+01 1.6642e+00
   21   std_len   9.6623e+01 1.7384e+00
   22   std_len   9.7069e+01 1.8042e+00
   23   std_len   9.7431e+01 1.8620e+00
   24   std_len   9.7726e+01 1.9125e+00
   25   std_len   9.7966e+01 1.9563e+00
   26   std_len   9.8160e+01 1.9941e+00
   27   std_len   9.8319e+01 2.0267e+00
```

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Parameter correlation from inverse hessian

vonb.cor — ADMB Course

vonB.tpl | vonb.rep | vonb.prf | vonB.dat | vonb.hst | vonb.par | lp_linf.plt | vonb.std | vonb.cor | vonBdem.R

```
The logarithm of the determinant of the hessian = 8.54727
index   name       value       std dev         1         2         3
    1   linf      9.9007e+01 2.2078e+00    1.0000
    2   k         2.0701e-01 1.1987e-02   -0.8502    1.0000
    3   lp_linf   9.9007e+01 2.2078e+00    1.0000   -0.8502    1.0000
```

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Likelihood profiles

- Declare a *likeprof_number* to carryout a likelihood profile.
- Implement with the -lprof command line option.
- Results are reported in a *.plt file for each *likeprof_* variable.

lp_linf.plt — ADMB Course

vonB.tpl | vonb.rep | vonb.prf | vonB.dat | vonb.hst | vonb.par | lp_linf.plt | vonb.std | vonb.cor | vonBdem.R

```
 3.61326 2.0022
 3.6176 1.93352
 3.62194 1.88274
 3.62628 1.83197
 3.63062 1.7812
 3.63496 1.73043
 3.6393 1.67966
 3.64364 1.62888
 3.64798 1.57811
Minimum width confidence limits:
 significance level  lower bound  upper bound
                              0.9              3.44667      3.60005
                             0.95              3.44628      3.62408
                            0.975              3.44589      3.63763

One sided confidence limits for the profile likelihood:

The probability is     0.9 that lp_linf is greater than 3.46321
The probability is    0.95 that lp_linf is greater than 3.45785
The probability is   0.975 that lp_linf is greater than 3.45417

The probability is     0.9 that lp_linf is less than 3.60022
The probability is    0.95 that lp_linf is less than 3.61994
The probability is   0.975 that lp_linf is less than 3.63245

Normal approximation
 3.4054 0.632449
 3.41195 1.23102
 3.4185 1.82959
```

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Markov Chain Monte Carlo (MCMC)

- Sampling of the likelihood surface to numerically approximate the joint posterior distribution.
- Two algorithms available:
  - Metropolis-hastings (-mcmc n)
  - a new Hybrid MCMC using Hamiltonian dynamics (-mcmc n -hybrid)
    - see Neal 2010 for more info

Metropolis-Hastings Algorithm

(1) Start Markov chain at modal estimate of $\hat{\Theta}$,

(2) take a random step from Θ_i to a new candidtate point Θ'_i,

(3) accept trail Θ'_i with probability: $\min\left[\frac{P(\Theta'_i)}{P(\Theta_i)}, 1\right]$,

(4) if Θ'_i is accepted it becomes the new point in the chain,
otherwise Θ_i is repeated,

(5) repeat steps 2-4 many many times.

3 samples

6 samples

20 samples

200 samples

1,500 samples

10,000 samples

Metabolic rate parameter (k)

Asymptotic length (cm)

0.24
0.22
0.20
0.18
0.16

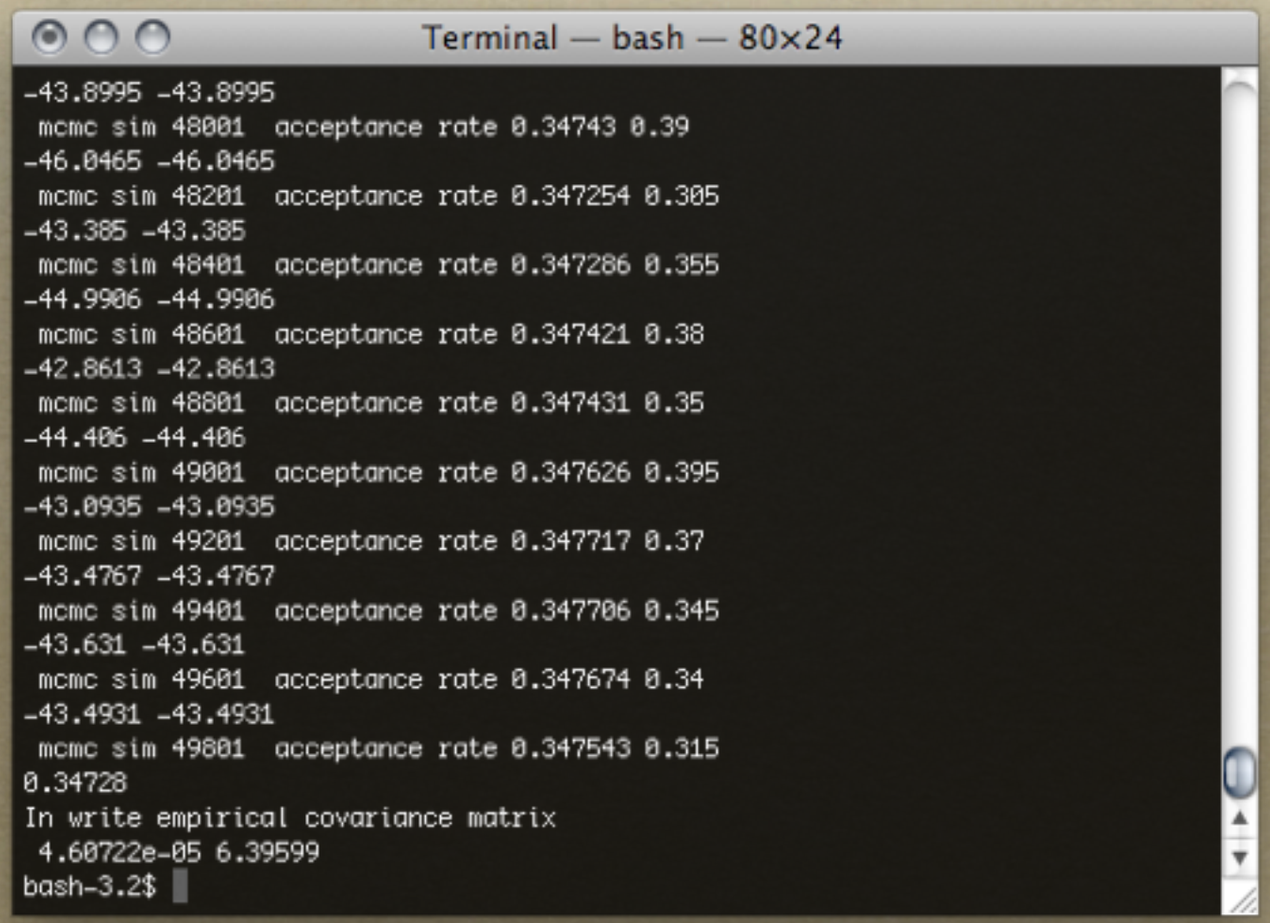
90
95
100
105
110

MCMC in AMDB

- To invoke the mcmc routines, you must have at least 1 sdreport_ variable
- Use the -mcmc n command line option to run in MCMC mode
- Use -mcsave n to save samples from the joint posterior distribution
- Use -mceval to run the model using posterior samples.

MCMC diagnostics & options

- monitor acceptance rate
- must have positive definite hessian matrix
- -mcseed # to repeat results
- see command line options -? for more options



Posterior density for L_{inf}