Specifying model parameters

AD Model Builder foundation

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PARAMETER_SECTION

- Is where model parameters should be specified
- Model parameters can be fixed at their initial values
- Bounds can be specified
- Phases can be specified (Start by estimating these, then include those, and so on)
- Additional variables for intermediate calculations, and additional outputs can be declared
- Finally the it should name the function to be minimized by a line like:
  `objective_function_value nll;`
- AD Model Builder will keep track of the derivatives for the quantities declared here

A single parameter

Unbounded, and active parameter: The most basic parameter is declared by:

```
init_number theta;
```

It is initialized to zero, if no other initialization is done (in program, or via a .pin file).

Bounded, and active parameter: Bounds are added by:

```
init_bounded_number p(0,1);
```

It is initialized to the mid-point of the interval (here 0.5), if no other initialization is done.

Fixed parameter: To fix a parameter at its initial value, simply add a '-1':

```
init_number theta(-1);
init_bounded_number p(0,1,-1);
```

Then its value will not be estimated.

Optimization in phases: In models with multiple parameters it is possible to have a parameter fixed during the first optimization (of some other parameters), and the active in the second or third. The phase from which it is set active ('1','2',or '3') is specified by:

`init_number theta(2);`	estimated in second phase
`init_bounded_number p(0,1,3);`	estimated in third phase

By default three phases are available, but more is possible (see ADMB manual).

Vectors of parameters

Unbounded, and always active: A vector with 3 elements and valid index from 1 to 3

```
init_vector theta(1,3);
```

It is initialized to zero by default

Bounded, and active: A vector with valid index from 0 to 5 and each element in]-1,3[

```
init_bounded_vector theta(0,5,-1,3);
```

It is initialized to the mid-point of the interval (here 1), if no other initialization is done.

Fixed: To fix all elements of a parameter vector we add a '-1' argument:

```
init_vector theta(1,3,-1);
init_bounded_vector theta(0,5,-1,3,-1);
```

Then they are kept at initialization.

Optimization in phases: The active optimization phase can be set for vectors too:

`init_vector theta(1,3,2);`	estimated in second phase
`init_bounded_vector theta(0,5,-1,3,3);`	estimated in third phase

By default three phases are available, but more is possible (see ADMB manual).

Parameter vector summing to zero: To declare a parameter vector that is optimized such that it sums to zero:

`init_bounded_dev_vector epsilon(1,20,-10,10,2)`

`init_dev_vector epsilon(1,20,2)`

Vectors of individual parameters: Consider the following example:

```
DATA_SECTION
  init_int N
  init_vector Y(1,N)
  init_vector x(1,N)
  init_vector lb(1,3)
  init_vector ub(1,3)
  init_ivector phase(1,3)

PARAMETER_SECTION
  init_bounded_number_vector th(1,3,lb,ub,phase)
  objective_function_value nll

PROCEDURE_SECTION
  nll=0.5*(N*log(2*M_PI*square(th(3)))
      +sum(square(Y-(th(1)+th(2)*x)))/square(th(3)));
```

```
# number of observations
     10
# observed Y values
    1.4  4.7  5.1  8.3  9.0  14.5
    14.0  13.4  19.2  18
# observed x values
    -1  0 1  2  3  4  5  6  7  8
# lower bounds a b sigma
  -100 -100 0
# upper bounds a b sigma
  100 100 100
# phase a b sigma
  1  1  2
```

```
The logarithm of the determinant of the hessian = 7.64036
index   name    value      std dev       1       2       3
    1   th[1]  4.0782e+00 7.0394e-01   1.0000
    2   th[2]  1.9091e+00 1.5547e-01  -0.7730  1.0000
    3   th[3]  1.4122e+00 3.1577e-01   0.0000  0.0000  1.0000
```

An unbounded version `init_number_vector` is also available.

Now we start to see a pattern

Declaration	type of object in DATA SECTION	type of object in PARAMETER SECTION
[init_]int	int	int
[init_][bounded_]number	double	dvariable
[init_][bounded_][dev_]vector	vector of doubles(dvector)	vector of dvariables(dvar_vector)
[init_][bounded_]matrix	matrix of doubles(dmatrix)	matrix of dvariables(dvar_matrix)
[init_]3darray	3 dimensional array of doubles	3 dimensional array of dvariables
4darray	4 dimensional array of doubles	4 dimensional array of dvariables
5darray	5 dimensional array of doubles	5 dimensional array of dvariables
6darray	6 dimensional array of doubles	6 dimensional array of dvariables
7darray	7 dimensional array of doubles	7 dimensional array of dvariables
sdreport_number	na	dvariable
sdreport_vector	na	vector of dvariables(dvar_vector)
sdreport_matrix	na	matrix of dvariables(dvar_matrix)

In the `PARAMETER_SECTION` the following rules apply:

- Everything starting with `init_` is optimized (unless phase is set to '-1').
- For everything starting with `sdreport_` AD Model Builder is instructed to estimate standard errors and correlations.
- Other `number`, `vector`, `matrix`, ... variables are used to store intermediate calculations

How are parameters initialized

- If none of the following methods are used, the default is to set unbounded parameters to **zero** and bounded parameters to the **interval midpoint**
- This default behaviour can be overruled by using the INITIALIZATION_SECTION as in:

```
PARAMETER_SECTION
  init_bounded_number_vector th(1,3,lb,ub,phase)
  objective_function_value nll
INITIALIZATION_SECTION
  th 1;
```

- Whatever is specified by default or in the INITIALIZATION_SECTION can be overwritten by supplying initial values in the <modelname>.pin file. Such a file could look like:

```
#th
4 2 1.5
```

  with the values appearing in the same order as the parameters in the PARAMETER_SECTION

- A final way to set initial values, which will overwrite all methods above is to use the PRELIMINARY_CALCS_SECTION as in:

```
PARAMETER_SECTION
  init_bounded_number_vector th(1,3,lb,ub,phase)
  objective_function_value nll
PRELIMINARY_CALCS_SECTION
  th(1)=2;
  th(2)=2;
  th(3)=2;
```

Transformations

- Bounded optimization in ADMB works great, but sometimes we need something different, or are in a situation where we prefer to a parameter transformation. Consider:

```
DATA_SECTION
  init_int N
  init_vector Y(1,N)
  init_vector x(1,N)

PARAMETER_SECTION
  init_number a
  init_number b
  init_number logSigma
  sdreport_number sigmasq
  objective_function_value nll

PROCEDURE_SECTION
  sigmasq=exp(2*logSigma);
  nll=0.5*(N*log(2*M_PI*sigmasq)+sum(square(Y-(a+b*x)))/sigmasq);
```

- We know σ must be positive, but we don't know the upper limit
- After estimation we want to supply a confidence interval. If we calculate it as $\sigma \in]\hat{\sigma} - 2\mathrm{sd}(\hat{\sigma}); \hat{\sigma} + 2\mathrm{sd}(\hat{\sigma})[$ it could get a negative lower bound.
- If we use the transformed variable $\xi = \log(\sigma)$ we get: $\sigma \in]e^{\hat{\xi}-2\mathrm{sd}(\hat{\xi})}; e^{\hat{\xi}+2\mathrm{sd}(\hat{\xi})}[$, which we know is entirely positive.

Probability vector

- For a single probability parameter we can use the inverse logit transformation

$$p = \exp(\alpha)/(1 + \exp(\alpha)), \quad \text{where } \alpha \in \mathcal{R}$$

- For a probability vector $p = (p_1, \ldots, p_n) \in]0,1[^n$ with $\sum p = 1$ we can use the following transformation:

$$p = \begin{pmatrix} \exp(\alpha_1)/(1 + \sum_{i=1}^{n-1} \exp(\alpha_i)) \\ \exp(\alpha_2)/(1 + \sum_{i=1}^{n-1} \exp(\alpha_i)) \\ \vdots \\ \exp(\alpha_{n-1})/(1 + \sum_{i=1}^{n-1} \exp(\alpha_i)) \\ 1 - \sum_{i=1}^{n-1} \exp(\alpha_i)/(1 + \sum_{i=1}^{n-1} \exp(\alpha_i)) \end{pmatrix} \quad \text{where } \alpha \in \mathcal{R}^{n-1}$$

- Example using a probability vector:

```
DATA_SECTION
  init_int dim;
  init_vector X(1,dim);

PARAMETER_SECTION
  init_vector a(1,dim-1);
  sdreport_vector p(1,dim);
  objective_function_value nll;

PROCEDURE_SECTION
  p=a2p(a);
  nll=-gammln(sum(X)+1.0)+sum(gammln(X+1.0))
      -sum(elem_prod(X,log(p)));

FUNCTION dvar_vector a2p(const dvar_vector& a)
  dvar_vector p(1,dim);
  dvar_vector expa=exp(a);
  p(1,dim-1)=expa/(1+sum(expa));
  p(dim)=1-sum(p(1,dim-1));
  return p;
```

```
6
 10 16 31 13 14 16
```

```
index   name   value        std dev
    1   a -4.7000e-01 4.0311e-01
    2   a  9.5044e-07 3.5355e-01
    3   a  6.6140e-01 3.0783e-01
    4   a -2.0764e-01 3.7339e-01
    5   a -1.3353e-01 3.6596e-01
    6   p  1.0000e-01 3.0000e-02
    7   p  1.6000e-01 3.6661e-02
    8   p  3.1000e-01 4.6249e-02
    9   p  1.3000e-01 3.3630e-02
   10   p  1.4000e-01 3.4699e-02
   11   p  1.6000e-01 3.6661e-02
```

Exercises

Exercise 1: Suggest how to use transformation to parametrize a parameter that is

a) only negative

b) between 2 and 5

c) an increasing vector

Solution: Consider the following transformations

a) $\theta = -e^{\alpha}, \quad$ where $\alpha \in \mathcal{R}$

b) $\theta = 3e^{\alpha}/(1 + e^{\alpha}) + 2, \quad$ where $\alpha \in \mathcal{R}$

c) $\theta = (e^{\alpha_1}, e^{\alpha_1} + e^{\alpha_2}, \ldots, e^{\alpha_1} + \cdots + e^{\alpha_n}), \quad$ where $\alpha \in \mathcal{R}^n$

Exercise 2: To investigate the effect of a certain type of exposure in three doses (1,2,and 3) the following experiment was carried out. The experimental unit was a cage with 2 rats. Once per month in 10 months the activity was measured as number of crossing of a light beam. The data can be seen on the next page. It must be expected that measurements from same cage are correlated, and even that measurements close in time have higher correlations.

The following model was proposed:

$$\log(\text{count}) \sim \mathcal{N}(\mu, \Sigma), \quad \text{where}$$

$$\mu_i = \alpha(\text{dose}_i, \text{month}_i), \quad i = 1 \ldots 300$$

$$\Sigma_{i,j} = \begin{cases} 0, & \text{if cage}_i \neq \text{cage}_j \\ \nu^2 + \tau^2 \exp\{\frac{-(\text{month}_i - \text{month}_j)^2}{\rho^2}\}, & \text{if cage}_i = \text{cage}_j \text{ and } i \neq j \\ \nu^2 + \tau^2 + \sigma^2, & \text{if } i = j \end{cases}$$

? Implement the model and remember that the variance parameters should be positive.

! The negative log density for the multivariate normal distribution is:

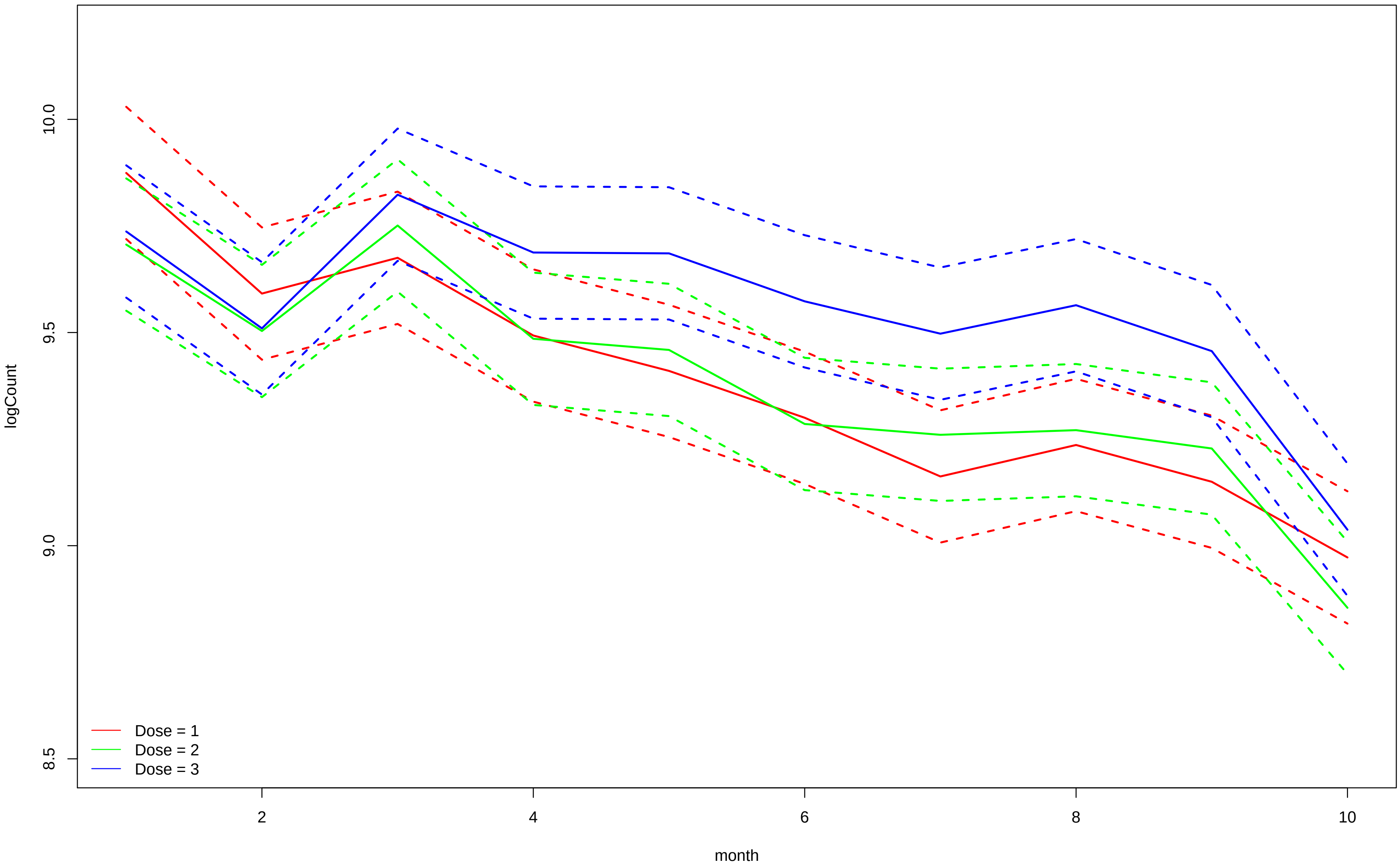
$$\ell(x, \mu, \Sigma) = \frac{1}{2}\left(N \log(2\pi) + \log|\Sigma| + (x - \mu)'\Sigma^{-1}(x - \mu)\right)$$

		Month									
Dose	Cage	1	2	3	4	5	6	7	8	9	10
1	1	20584	15439	17376	14785	11189	10366	8725	9974	9576	6849
1	2	23265	16956	16200	12934	13763	11893	9949	10490	8674	7153
1	3	17065	12429	14757	10524	11783	8828	9016	9635	8028	8099
1	4	19265	19316	20598	16619	16092	13422	10532	10614	9466	9494
1	5	21062	14095	13267	12543	12734	12268	12219	11791	10379	8463
1	6	23456	10939	13270	14089	12986	13723	11878	13338	12442	10094
1	7	13383	11899	12531	15081	14295	13650	9988	11518	11915	7844
1	8	22717	22434	23151	13163	10029	10408	9119	10188	9549	11153
1	9	17437	13950	15535	14199	11540	9568	8481	9143	8117	5765
1	10	18546	12520	15394	10137	9218	7343	6702	7173	7257	5708
2	11	18536	16827	19185	12445	13227	10412	9855	9169	9639	6853
2	12	18831	14043	16493	12562	10397	8568	8599	8818	6011	5062
2	13	15016	13765	16648	14537	13929	10778	9897	9225	9491	5523
2	14	22276	15497	22024	15616	12440	11454	10290	9456	9567	7003
2	15	18943	14834	18403	16232	13085	12679	10489	9495	10896	8836
2	16	13598	10233	13392	10457	9236	8847	9445	9501	8509	5656
2	17	20498	22136	22094	19825	18157	11452	14809	14564	14503	10643
2	18	19586	12710	12745	7294	15757	15296	14097	14308	13933	10210
2	19	11474	8108	17714	16795	17364	16766	15016	13475	14349	8698
2	20	10284	10760	15628	10692	8420	5842	6138	10271	8435	4486
3	21	18459	15805	19924	18337	24197	18790	19333	22234	18291	11595
3	22	16186	11750	16470	18637	14862	14695	14458	14228	12909	9079
3	23	9614	8319	11375	9446	13157	11153	10540	11476	8976	6123
3	24	15688	15016	20929	12706	17351	15089	14605	15952	14795	10434
3	25	15864	13169	20991	20655	19763	19180	19003	18172	15025	11790
3	26	17721	14489	19085	21333	17011	16148	15280	14762	15745	10477
3	27	17606	7558	15646	15194	13036	10316	8172	8977	8378	3962
3	28	34907	29247	35831	15093	9754	10061	9042	11732	8716	4922
3	29	15189	14046	14909	14713	14999	14201	13184	13073	14639	10330
3	30	16388	14538	17548	19416	22034	17761	14488	16068	14773	10595

```
#noCages
30
#noMonths
10
# month
1 2 3 4 5 6 7 8 9 10
# dose
1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3
# cage
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
# counts
20584  15439  17376  14785  11189  10366  8725   9974   9576   6849
23265  16956  16200  12934  13763  11893  9949   10490  8674   7153
17065  12429  14757  10524  11783  8828   9016   9635   8028   8099
19265  19316  20598  16619  16092  13422  10532  10614  9466   9494
21062  14095  13267  12543  12734  12268  12219  11791  10379  8463
23456  10939  13270  14089  12986  13723  11878  13338  12442  10094
13383  11899  12531  15081  14295  13650  9988   11518  11915  7844
22717  22434  23151  13163  10029  10408  9119   10188  9549   11153
17437  13950  15535  14199  11540  9568   8481   9143   8117   5765
18546  12520  15394  10137  9218   7343   6702   7173   7257   5708
18536  16827  19185  12445  13227  10412  9855   9169   9639   6853
18831  14043  16493  12562  10397  8568   8599   8818   6011   5062
15016  13765  16648  14537  13929  10778  9897   9225   9491   5523
22276  15497  22024  15616  12440  11454  10290  9456   9567   7003
18943  14834  18403  16232  13085  12679  10489  9495   10896  8836
13598  10233  13392  10457  9236   8847   9445   9501   8509   5656
20498  22136  22094  19825  18157  11452  14809  14564  14503  10643
19586  12710  12745  7294   15757  15296  14097  14308  13933  10210
11474   8108  17714  16795  17364  16766  15016  13475  14349  8698
10284  10760  15628  10692  8420   5842   6138   10271  8435   4486
18459  15805  19924  18337  24197  18790  19333  22234  18291  11595
16186  11750  16470  18637  14862  14695  14458  14228  12909  9079
9614    8319  11375  9446   13157  11153  10540  11476  8976   6123
15688  15016  20929  12706  17351  15089  14605  15952  14795  10434
15864  13169  20991  20655  19763  19180  19003  18172  15025  11790
17721  14489  19085  21333  17011  16148  15280  14762  15745  10477
17606   7558  15646  15194  13036  10316  8172   8977   8378   3962
34907  29247  35831  15093  9754   10061  9042   11732  8716   4922
15189  14046  14909  14713  14999  14201  13184  13073  14639  10330
16388  14538  17548  19416  22034  17761  14488  16068  14773  10595
```

Solution: The following program implements the model

```
DATA_SECTION
  init_int noCages
  init_int noMonths
  init_ivector month(1,noMonths)
  init_ivector dose(1,noCages)
  init_ivector cage(1,noCages)
  init_matrix counts(1,noCages,1,noMonths)
  matrix lc(1,noCages,1,noMonths)
  !!  lc=log(counts);

PARAMETER_SECTION
  init_matrix DxM(1,3,1,noMonths);
  init_number logNu;
  init_number logTau;
  init_number logSigma;
  init_number logRho;

  sdreport_number nu2;
  sdreport_number tau2;
  sdreport_number sigma2;
  sdreport_number rho2;

  objective_function_value nll;

PROCEDURE_SECTION
  nu2=exp(2*logNu);
  tau2=exp(2*logTau);
  sigma2=exp(2*logSigma);
  rho2=exp(2*logRho);

  dvar_matrix S(1,noMonths,1,noMonths);
  for(int i=1; i<=noMonths; ++i){
    S(i,i)=nu2+tau2+sigma2;
    for(int j=i+1; j<=noMonths; ++j){
      S(i,j)=nu2+tau2*exp(-square(month(i)-month(j))/rho2);
      S(j,i)=S(i,j);
    }
  }
  dvar_matrix Sinv=inv(S);
  dvariable logdet=log(det(S));

  nll=0.0;
  for(int i=1; i<=noCages; ++i){
    nll+=mvdnormi(lc(i),DxM(dose(i)),Sinv,logdet);
  }

FUNCTION dvariable mvdnormi(const dvector& x, const dvar_vector& mu, const dvar_matrix& Sinv, const dvariable& logdet)
  dvar_vector diff=x-mu;
  return 0.5*(log(2.0*M_PI)*noMonths+logdet+diff*Sinv*diff);
```



logCount
month
Dose = 1
Dose = 2
Dose = 3
10.0
9.5
9.0
8.5
2
4
6
8
10