9 Learning Algorithms

CONTENTS

In this chapter we present two classes of learning algorithms. We begin with the genetic algorithm, which lends itself well to many statistical modeling and optimization problems, such as variable subsetting, mixture modeling, and maximum likelihood estimation. After that we detail a function implementing simulated annealing, though it does not seem as valuable a statistical modeling tool as the genetic algorithm.

9.1 Introduction

The first part of this chapter is dedicated to the genetic algorithm; the value of this optimization technique is demonstrated in two contexts - variable subsetting and maximum likelihood estimation. The genetic algorithm (GA) is a stochastic search procedure that borrows concepts from biological evolution. Biological chromosomes, which determine so much about organisms, are represented as binary words – these determine the composition of possible solutions to an optimization problem. As an

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example, consider a subsetting problem such as would occur in multivariate regression: each solution is a q-length vector such that each locus represents the presence (1) or absence (0) of a specific predictor. An example may be $\left[1\ 0\ 0\ 1\ 1\ 0\ 0\ 1\right]$; in this case, predictors 1,4,5,8 will be used for OLS while 2,3,6,7 will not. In the context of a numerical optimization problem, the chromosomes represent a real value. Consider the problem of finding the MLE for some single parameter distribution where we have reason to believe the maximum $\hat{\theta}$ lies in the interval (θ_L, θ_U). We can use this information to encode real values in this range as binary chromosomes. For example, say our interval is $(-10, 10)$, and we want to use $B = 8$ bits. The real value $x = 3.6$ would be encoded as $\left[1\ 0\ 1\ 0\ 1\ 1\ 0\ 1\right]$.

Each iteration of the GA is called a *generation*; maintaining the biological analogy, each generation is composed of a *population* of solutions called *individuals* - all represented by binary *chromosomes*. Within a generation, individuals are allowed to perpetuate their genes by mating; with whom they mate, and the frequency with which they mate is determined by their *fitness* as defined by some *objective function*. Unlike the biological analogy, mating always produces two offspring, so the population remains of a constant size (more this paragraph). When two individuals mate, there is a certain probability that their chromosomes will trade portions, through a *crossover* operation; this probability is usually set rather high (0.75 for example). When members of the current generation procreate, there is a typically small probability (0.10 for example) that some spots (*loci*) on the offspring's chromosomes will *mutate*: $1 \longrightarrow 0$ or $0 \longrightarrow 1$. The benefit of the mutation operator should be clear, without it, the GA would suffer from the main pitfall of most search procedures: that of getting stuck in local optimum. Even if a next generation ended up completely homogenous after crossover, mutation would widen the search by allowing a jump to another area of the fitness landscape. In real life, it can occasionally happen that an especially fit individual will remain a desirable partner for more than one generation; think Sean Connery, Harrison Ford, or Charlton Heston. In the genetic algorithm, members of a current generation generally die after procreation, leaving the next generation all offspring. However, if the *elitism* rule is on, the most fit solution from the current generation does not die, but remains to mate with the ensuing generation. Note that this means the population will grow with each generation. The final (and more recently developed) operation is called *GA engineering* operation. The biological analogue would be that of a virus that inserts a section of it's DNA into a host's DNA; in this context, the inserted bits code the difference between the most fit individuals of the current and previous generations. As in real life, this virus infects individuals with a certain probability that is set by the researcher.

Setting the number of generations and population size is largely subjective. In the subsetting case, the general rule of thumb for selecting the size of the population is that it should be larger than the number of variables. The researcher can experiment with these two parameters on the same dataset to get a feel for where to set them. If either is too large, the computational burden can increase rapidly. However, if they are too small, the GA may finish with a suboptimal solution. Consider a situation in which the number of generations is set to 100, but the procedure found the optimal solution in generation 20. If the objective function can't improve anymore, there's no reason to waste the computation time to go 80 more generations. Thus, we allow for premature termination with a 3rd parameter. If the GA has iterated through some number of generations with no improvement in the best score, we consider it to have converged, and quit. In our example here, if the premature termination threshold was set to 40, the GA would quit early in generation 59 - saving a substantial amount of computation time. Thus, the general algorithm is simple and straightforward:

1. Generate initial population of chromosomes - this is usually done randomly.
2. Score all members of current population.
3. Check early termination criteria.
4. Determine how current population is mated and represented in next generation.
5. Perform chromosomal crossover, genetic mutation, and GA engineering.
6. Allow current generation to die off, except the best individual if elitism is on, then pass on offspring to new generation.
7. Loop back to *Step 2* until termination criteria met.

See *Chapter 23 - Multivariate Mixture Model Cluster Analysis* for details of the M^3 subtoolbox which implements the genetic algorithm in the mixture modeling context. The MultVarRegGASub subtoolbox, introduced in *Chapter 13 - Multivariate Regression*, uses the GA to find optimal subset regression models under both correctly specified and misspecified models. Both implementations utilize a class of objective functions called Information Criteria.

We finish the chapter with a function that implements Adaptive Simulated Annealing for the maximum likelihood estimation problem. The way Simulated Annealing (SA) works to find a minimum of a p-dimensional function is similar to the way the cooling of a molten metal is controlled so as to increase the size of its crystals. The latent heat liberates the atoms from their local minima and wander randomly through states of higher energy; the controlled cooling gives the material more chances of finding configurations with lower internal energy. The function to minimize represents the internal energy; there are different methods for computing the cooling schedule from a high temperature to a low temperature. The general algorithm is:

1. Set initial state and temperature, compute initial energy.
2. Update temperature, find neighboring state to consider, and compute it's energy.
3. If energy is lower, move current state. If energy is higher, move current state with some probability dependent upon the cost and current temperature.
4. Update time step, then loop back to *Step 2* until termination criteria met.

General Files	
SimDistData	General function for simulating from various densities.
ComputePDF	General function for computing PDFs of various densities.
ComputeLogLike	General function for computing the log likelihood of various densities.
EstParamRanges	General function for estimating parameter ranges for various densities.
Genetic Algorithm Files	
GA10to2	Encode real (base 10) numbers as binary (base 2).
GA2to10	Decode binary numbers into real.
GAselect	Use fitness scores to prepare a generation for mating.
GAcrossover	Mate members of a generation as prepared by GAselect.
GAmutation	Perform random mutation on a generation.
GAengineering	Insert bits into next generation.
GArealoptim	GA for optimization of real-valued functions.
GAtemplate	Generic template for subsetting problems with the GA.
drv_GAMLE	Script that finds MLEs for various densities using the real-valued GA.
Simulated Annealing Files	
SimAnneal_MLE	Use Simulated Annealing to find MLEs.

TABLE 9.1
Functions and Scripts.

9.2 General Data Simulator

Syntax

[data, state] = SimDistData(distribution, sample size, parameters, state)

Description

This is a general function for simulating data, it calls other Matlab random generators. The exponential distribution uses the avg. lifetime parameterization: $f(x) = \frac{1}{b} exp\left(-\frac{x}{b}\right) = exppdf(x,b)$. The gamma has $\frac{1}{b}$ instead of the usual b: $f(x) = \frac{x^{a-1} exp\left(-\frac{x}{b}\right)}{b^a \Gamma(a)} = gampdf(x,a,b)$. The weibull has a^{-b} instead of the usual a: $f(x) = abx^{b-1} exp(-ax^b) = weibpdf(x,a,b)$. As should be clear, this function has nothing to do with the genetic algorithm. However, it is here because it is used by the drv_GAMLE script, discussed later, to demonstrate use of the real-valued genetic algorithm.

Input / Output

- distribution - Character code indicating distribution to use:

UNI $= U(0,b)$	NRM $= N(\mu,\sigma)$
GAM $= Gam(a,b)$	LOG $= LogN(\mu,\sigma)$
EXP $= Exp(b)$	WEI $= Weib(a,b)$
CHI $= \chi^2(\nu)$	BET $= Beta(a,b)$
STU $= t(\nu)$	CAU $= Cauchy(\theta)$
LPL $= Laplace(\mu,\sigma)$	PXP $= PEXP(\mu,\sigma,\beta)$
PAR $= Pareto(c)$	F $= F(\nu_1,\nu_2)$

- sample size - Scalar number of observations required.
- parameters - Appropriately sized vector holding parameters for specified distribution.
- state - Optional scalar randomizer state: -1 = no randomization, 0 = use sum(clock*1000000) (default), else = actual state to use.
- data - $(n \times 1)$ vector of random data.
- state - Randomizer state used, if set.

If no arguments are passed in, this function returns two special lists. The data parameter will hold a 2d cell array with distribution codes in the first column and parameter names in the second column. The state parameter will have a 2d matrix with the number of parameters for each distribution in the 1st column. The second column holds range support codes for the distributions: $1 =$ strictly nonnegative, $0 =$ entire real line.

Algorithm

With the exception of the Cauchy, Pareto, and power exponential distributions, SimDistData just calls the appropriate random number generators included in the Matlab Statistics Toolbox. For the Cauchy and Pareto distributions, random variates are generated using the inverse CDF method. First, *n* random variates (called *p*) are generated from the uniform distribution. Using these, the samples are computed as:

$$\text{Cauchy: } t = \tan\left(\pi p + \arctan\left(-\infty - \theta\right)\right) + \theta, \tag{9.1}$$

$$\text{Pareto: } t = (1-p)^{-\frac{1}{c}} - 1. \tag{9.2}$$

For the power exponential distribution, we implement an iterative procedure in which a sample *t* is accepted if

$$\sqrt{\sigma^2}\exp\left(-\frac{1}{2}\left[\frac{(t-\mu)^2}{\sigma^2}\right]^{\beta}\right) \geq p_2, \text{ for}$$
$$t = 8\sigma^2 p_1 + \mu - 4\sigma^2. \tag{9.3}$$

Example

The following code was used to generate the two plots in *Figure 9.1*.

```
fig = figure('units','inches');
% generate and plot Chi^2(3) data
X1 = SimDistData('CHI',5000,3,42);
subplot(1,2,1),[e,c,f] = DensityHist(X1,15,1);
[x1,y1] = ComputePDF('CHI',3,[e(1),e(end)]);
hold on, plot(x1,y1,'r'),hold off
title('Sim Data with \chi^2(3) Density Overlay')
% generate and plot standard normal data
X2 = SimDistData('NRM',5000,[0,1],42);
subplot(1,2,2),[e,c,f] = DensityHist(X2,15,1);
[x2,y2] = ComputePDF('NRM',[0,1],[e(1),e(end)]);
hold on, plot(x2,y2,'r'),hold off
title('Sim Data with N(0,1) Density Overlay')
loc = get(fig,'position');
set(fig,'position',[loc([1,2]),6.25,3])
```

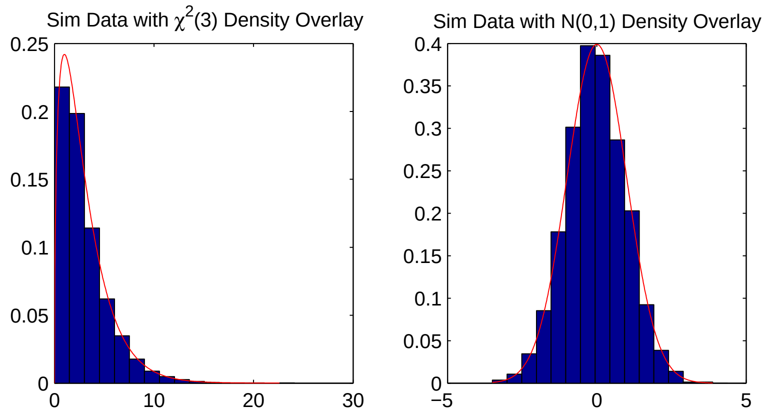


FIGURE 9.1: Simulated Data with Theoretical Density Overlays.

9.3 General Density Plotter

Syntax

[x,y] = ComputePDF(distribution, parameters, data min and max)

Description

This is a general function for computing the densities with respect to a specified distribution, for some data, such that the range output in x encompasses the data and the distribution. This is particularly useful for doing a density histogram for some data with a theoretical distribution overlaying it. Note that though you can generate uniform, beta, or F data with SimDistData, this function can't compute the density for them. The exponential distribution uses the avg. lifetime parameterization: $f(x) = \frac{1}{b} exp\left(-\frac{x}{b}\right) = exppdf(x,b)$. The gamma has $\frac{1}{b}$ instead of the usual b: $f(x) = \frac{x^{a-1} exp\left(-\frac{x}{b}\right)}{b^a \Gamma(a)} = gampdf(x,a,b)$. The weibull has a^{-b} instead of the usual a: $f(x) = abx^{b-1} exp(-ax^b) = weibpdf(x,a,b)$. As should be clear, this function has nothing to do with the genetic algorithm. However, it is here because it is used by the drv_GAMLE script, discussed later, to demonstrate use of the real-valued genetic algorithm.

Input / Output

- distribution - Character code indicating distribution to use:

NRM $= N(\mu,\sigma)$	GAM $= Gam(a,b)$
LOG $= LogN(\mu,\sigma)$	EXP $= Exp(b)$
WEI $= Weib(a,b)$	CHI $= \chi^2(\nu)$
STU $= t(\nu)$	CAU $= Cauchy(\theta)$
LPL $= Laplace(\mu,\sigma)$	PXP $= PEXP(\mu,\sigma,\beta)$
PAR $= Pareto(c)$	

- parameters - Appropriately sized vector holding parameters for specified distribution.
- data min and max - (1×2) vector holding the range of the data.
- x - (100×1) vector of plotting range.
- y - (100×1) vector of densities for x.

Algorithm

For most of the distributions included, ComputePDF used the quantile and pdf functions that come in the Matlab Statistics toolbox. The ranges are estimated using the 0.5^{th} and 99.5^{th} percentiles. As with SimDistData, the exceptions are the Cauchy, Pareto, and power exponential distributions. For the latter, the range is assumed to be $[-6,6]$. The ranges for the other two are computed using the quantile functions shown in *equations 9.1* and *9.2*. The density estimates are computed using the following two equations.

$$\text{Cauchy: } y = \frac{1}{\pi\left(1+(x-\theta)^2\right)}, \tag{9.4}$$

$$\text{Pareto: } y = \frac{c}{(1+x)^{c+1}}. \tag{9.5}$$

Example

The following code demonstrates using ComputePDF by plotting the χ^2, standard normal, and laplace densities all on the same graph in *Figure 9.2*.

```
[x1,y1] = ComputePDF('CHI',3,[0,10]);
[x2,y2] = ComputePDF('NRM',[0,1],[-4,4]);
[x3,y3] = ComputePDF('LPL',[2,0.5],[-4,4]);
plot(x1,y1,'r.-',x2,y2,'bs-',x3,y3,'gx-')
legend('\chi^2(3)','N(0,1)','LAPL(2,2)')
```

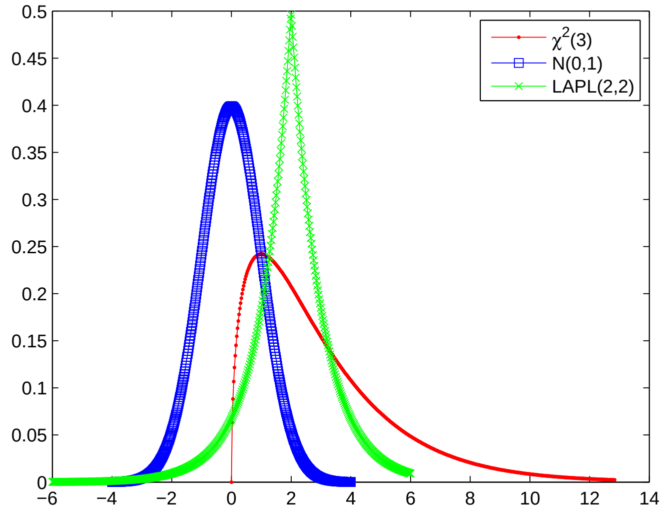


FIGURE 9.2: χ^2, Standard Normal, and Laplace Densities.

9.4 General Log Likelihood Computer

Syntax

log likelihood = ComputeLogLike(parameters, data, distribution)

Description

This is a general function for computing the log likelihood with respect to a specified distribution, for some data. Note that though you can generate uniform, beta, or F data with SimDistData, this function can't compute the log likelihood for fitting those distributions. The exponential distribution uses the avg. lifetime parameterization: $f(x) = \frac{1}{b} exp\left(-\frac{x}{b}\right) = exppdf(x,b)$. The gamma has $\frac{1}{b}$ instead of the usual b: $f(x) = \frac{x^{a-1} exp\left(-\frac{x}{b}\right)}{b^a \Gamma(a)} = gampdf(x,a,b)$. The weibull has a^{-b} instead of the usual a: $f(x) = abx^{b-1} exp(-ax^b) = weibpdf(x,a,b)$. As should be clear, this function has nothing to do with the genetic algorithm. However, it is here because it is used by the drv_GAMLE script, discussed later, to demonstrate use of the real-valued genetic algorithm.

Input / Output

- parameters - Appropriately sized vector holding parameters for specified distribution.
- data - $(n \times 1)$ vector of data.
- distribution - Character code indicating distribution to use:

NRM $= N(\mu,\sigma)$	GAM $= Gam(a,b)$
LOG $= LogN(\mu,\sigma)$	EXP $= Exp(b)$
WEI $= Weib(a,b)$	CHI $= \chi^2(\nu)$
STU $= t(\nu)$	CAU $= Cauchy(\theta)$
LPL $= Laplace(\mu,\sigma)$	PXP $= PEXP(\mu,\sigma,\beta)$
PAR $= Pareto(c)$	

- log likelihood - Scalar log likelihood value computed at parameters with data.

If no arguments are passed in, this function returns two special lists. The log likelihood parameter will hold a 2d cell array with distribution codes in the first column and parameter names in the second column. A second parameter will have a 2d matrix with the number of parameters for each distribution in the 1st column. The second column holds range support codes for the distributions: $1 =$ strictly nonnegative, $0 =$ entire real line.

Algorithm

The log likelihood for the all distributions are computed as shown in *Table 9.2*. The log likelihood for the Laplace is computed using the Power Exponential with $\beta = 0.5$.

Normal	$-\frac{1}{2}n\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$
Gamma	$-n\log\left(b^a\Gamma(a)\right) + (a-1)\sum_{i=1}^{n}\log(x_i) - \frac{1}{b}\sum_{i=1}^{n}x_i$
LogNormal	$-\frac{1}{2}n\log\left(2\pi\sigma^2\right) - \sum_{i=1}^{n}\log(x_i) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(\log(x_i)-\mu)^2$
Exponential	$-n\log(b) - \frac{1}{b}\sum_{i=1}^{n}x_i$
Weibull	$n\log\left(ba^{-b}\right) + (b-1)\sum_{i=1}^{n}\log(x_i) - a^{-b}\sum_{i=1}^{n}x_i^b$
χ^2	$-n\log\left(\Gamma\left(\frac{\nu}{2}\right)2^{\frac{\nu}{2}}\right) + \left(\frac{\nu}{2}-1\right)\sum_{i=1}^{n}\log(x_i) - \frac{1}{2}\sum_{i=1}^{n}x_i$
Student's t	$n\log\left(\frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\pi\nu}\Gamma\left(\frac{\nu}{2}\right)}\right) - \frac{\nu+1}{2}\sum_{i=1}^{n}\log\left(1+\frac{x_i^2}{\nu}\right)$
Cauchy	$-n\log(\pi) - \sum_{i=1}^{n}\log\left(1+(x_i-\theta)^2\right)$
Power Exponential	$-n\log\left(\sigma\Gamma\left(1+\frac{1}{2\beta}\right)2^{1+\frac{1}{2\beta}}\right) - \frac{1}{2}\sum_{i=1}^{n}\left\lvert\frac{x_i-\mu}{\sigma}\right\rvert^{2\beta}$
Pareto	$n\log(c) - (c+1)\sum_{i=1}^{n}\log(1+x_i)$

TABLE 9.2
Log Likelihood Functions

Example

The Matlab code here computes the log likelihood for discrete values $x = 1, \ldots, 10$ for both the standard normal distribution and the χ^2 distribution with $\nu = 3$ degrees of freedom. In both cases, note that the log likelihood, as computed by the ComputeLogLike function matches that as computed by the definition $\log l(\theta) = \prod_{i=1}^{n} f(x_i \mid \theta)$. Also, note that, under the principle of likelihood maximization, the $\chi^2(3)$ seems more likely for this data than $N(0,1)$. This make sense - the 99th percentile for the standard normal is only 2.326.

```
INPUT
x = [1:1:10];
mu = 0; sigma = 1; nu = 3;
ll1 = ComputeLogLike([mu,sigma],x,'NRM');
ll2 = log(prod(normpdf(x,mu,sigma)));
disp('Normal Log Likelihood')
disp(sprintf('From ComputeLogLike: %0.4f',ll1))
disp(sprintf('Using Definition: %0.4f',ll2))
disp('--------------------')
ll1 = ComputeLogLike(nu,x,'CHI');
ll2 = log(prod(chi2pdf(x,nu)));
disp('ChiSquared Log Likelihood')
disp(sprintf('From ComputeLogLike: %0.4f',ll1))
disp(sprintf('Using Definition: %0.4f',ll2))
OUTPUT
Normal Log Likelihood
From ComputeLogLike: -201.6894
Using Definition: -201.6894
--------------------
ChiSquared Log Likelihood
From ComputeLogLike: -29.1372
Using Definition: -29.1372
```

9.5 General Parameter Range Estimator

Syntax

[lower bound(s), upper bound(s)] = EstParamRanges(distribution, data)

Description

This is a general function for computing the possible ranges for the parameters of various distributions. For the Gamma distribution, this calls the MLE function in the Matlab statistics toolbox. The exponential distribution uses the avg. lifetime parameterization: $f(x) = \frac{1}{b} exp\left(-\frac{x}{b}\right) = exppdf(x,b)$. The gamma has $\frac{1}{b}$ instead of the usual b: $f(x) = \frac{x^{a-1} exp\left(-\frac{x}{b}\right)}{b^a \Gamma(a)} = gampdf(x,a,b)$. The weibull has a^{-b} instead of the usual a: $f(x) = abx^{b-1} exp(-ax^b) = weibpdf(x,a,b)$. As should be clear, this function has nothing to do with the genetic algorithm. However, it is here because it is used by the drv_GAMLE script, discussed later, to demonstrate use of the real-valued genetic algorithm.

Input / Output

- distribution - Character code indicating distribution to use:

NRM $= N(\mu,\sigma)$	GAM $= Gam(a,b)$
LOG $= LogN(\mu,\sigma)$	EXP $= Exp(b)$
WEI $= Weib(a,b)$	CHI $= \chi^2(\nu)$
STU $= t(\nu)$	CAU $= Cauchy(\theta)$
LPL $= Laplace(\mu,\sigma)$	PXP $= PEXP(\mu,\sigma,\beta)$
PAR $= Pareto(c)$	

- data - $(n \times 1)$ vector of data.
- lower bound(s) - $(1 \times p)$ vector holding lower bounds for the parameters of the distribution.
- upper bound(s) - $(1 \times p)$ vector holding upper bounds for the parameters of the distribution.

Algorithm

The methods used to compute the probable ranges for the parameters can be seen in *Table 9.3*. Here, $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{X})^2$; likewise, $\bar{X}_{\log} = \frac{1}{n}\sum_{i=1}^{n}\log(x_i)$ and $S^2_{\log} = \frac{1}{n-1}\sum_{i=1}^{n}(\log(x_i) - \bar{X})^2$. Several methods work by building a sort of confidence interval, while others build an interval around something like a method-of-moments estimator.

Example

We demonstrate this function by generating $n = 50$ random samples from three distributions $\chi^2(3)$, $Weibull\left(2, \frac{1}{2}\right)$, $PEXP(-2, 1.5, 2)$. Hence we evaluate the effectiveness on a single-, double, and triple- parameter distributions. As you can see, for all three distributions, the parameters all lie in the estimated ranges.

Normal	$\mu \in \left(\bar{X} \pm 2\frac{S}{\sqrt{n}}\right), \sigma \in (0.0001, 1.5S)$
Gamma	$a \in [0.5, 1.5]\,\hat{a}, b \in [0.5, 1.5]\,\hat{b}$
LogNormal	$\mu \in \left(\bar{X}_{\log} \pm 2\frac{S_{\log}}{\sqrt{n}}\right), \sigma \in (0.0001, 1.5S)\log$
Exponential	$b \in \left(\bar{X} \pm 2\frac{\bar{X}^2}{\sqrt{n}}\right)$
Weibull	$a \in \left(0.5\frac{1}{\bar{X}}, 1.5\frac{1}{\bar{X}}\right), b \in \left(0.0001, 1.5\frac{1}{S}\right)$
χ^2	$\nu \in \left(0, 2\frac{2\bar{X}}{\sqrt{n}}\right)$
Student's t	$\nu \in \left(0, \left\lvert 1.5\frac{-2S^2}{1-S^2}\right\rvert\right)$
Cauchy	$\theta \in \left(\bar{X} \pm 2\frac{S}{\sqrt{n}}\right)$
Laplace	$\mu \in \left(\bar{X} \pm 2\frac{S}{\sqrt{n}}\right), \sigma \in (0.0001, 1.5S)$
Power Exponential	$\mu \in \left(\bar{X} \pm 2\frac{S}{\sqrt{n}}\right), \sigma \in (0.0001, 1.5S), \beta \in (0.1, 5)$
Pareto	$c \in \left(0, 1.5\frac{n}{\sum_{i=1}^{n}\log(1+x_i)}\right)$

TABLE 9.3
Range Calculation Methods

```
INPUT
rand('state',42)
n = 50;
% chi-squared distribution
CHI_parm = 4;
X_CHI = SimDistData('CHI',n,CHI_parm);
[CHI_l,CHI_u] = EstParamRanges('CHI',X_CHI);
CHI_parmin = sum((CHI_parm >= CHI_l) + (CHI_parm <= CHI_u))/2;
if CHI_parmin == length(CHI_parm)
    disp('CHI: True Param(s) Lie(s) in Range')
else
    disp('CHI: True Param(s) Lie(s) out of Range')
end
disp(table2str({'nu'},[CHI_parm;CHI_l;CHI_u],{'%0.4f'},...
    0,{'TRUE';'L';'U'}))
% weibull distribution
WEI_parm = [2,0.5];
X_WEI = SimDistData('WEI',n,WEI_parm);
[WEI_l,WEI_u] = EstParamRanges('WEI',X_WEI);
WEI_parmin = sum((WEI_parm >= WEI_l) + (WEI_parm <= WEI_u))/2;
if WEI_parmin == length(WEI_parm)
    disp('WEI: True Param(s) Lie(s) in Range')
else
    disp('WEI: True Param(s) Lie(s) out of Range')
```

```
end
disp(table2str({'a';'b'},[WEI_parm;WEI_l;WEI_u],{'%0.4f'},...
    0,{'TRUE';'L';'U'}))
% power exponential distribution
PXP_parm = [-2,1.5,2];
X_PXP = SimDistData('PXP',n,PXP_parm);
[PXP_l,PXP_u] = EstParamRanges('PXP',X_PXP);
PXP_parmin = sum((PXP_parm >= PXP_l) + (PXP_parm <= PXP_u))/2;
if PXP_parmin == length(PXP_parm)
    disp('PXP: True Param(s) Lie(s) in Range')
else
    disp('PXP: True Param(s) Lie(s) out of Range')
end
disp(table2str({'mu','sigma','beta'},[PXP_parm;PXP_l;...
    PXP_u],{'%0.4f'},0,{'TRUE';'L';'U'}))
OUTPUT
CHI: True Param(s) Lie(s) in Range
------------
       nu
------------
TRUE 4.0000
L    0.0000
U    6.0665
------------
WEI: True Param(s) Lie(s) in Range
-------------------
        a      b
-------------------
TRUE 2.0000 0.5000
L    1.2792 0.0001
U    3.8377 2.0237
-------------------
PXP: True Param(s) Lie(s) in Range
---------------------------
         mu    sigma  beta
---------------------------
TRUE -2.0000 1.5000 2.0000
L    -2.4088 0.0001 0.1000
U    -1.7720 1.6886 5.0000
---------------------------
```

9.6 Real to Binary Conversion

Syntax

binary values = GA10to2(real values, number bits, lower bounds, upper bounds);

Description

Convert a vector of real values into a binary vector that can be operated on by the genetic algorithm. The values can be decoded using GA2to10

Input / Output

- real values - $(1 \times p)$ vector holding real values to encode as a single binary vector.
- number bits - $(1 \times p)$ vector with number of bits used to encode each real value.
- lower bounds - $(1 \times p)$ vector with lower bound of range for each real value.
- upper bounds - $(1 \times p)$ vector with upper bound of range for each real value.
- binary values - $(1 \times sum(\text{number bits}))$ vector binary string encoding all p real values.

Algorithm

For each element of real values, R, the entire allowable range is divided into steps using the formula

$$S = \frac{\max - \min}{2^B - 1}, \tag{9.6}$$

where B is the number of bits used to encode that value. The number of steps required for the actual value are then computed as

$$N = \frac{R - \min}{S}. \tag{9.7}$$

The Matlab function dec2bin is then used to encode the value of N in at least B bits.

Example

First we demonstrate the importance of using enough bits to encode a value. Let us consider an allowable range of $[-100,100]$, and attempt to use 2 bits to encode the real value of 90. Here we see that one byte was clearly not enough to perform the encoding - the binary string $[1,0]$ was decoded using the same range, it got 33.33. However, if we use 16 bits, we get a very close decimal value back. If we used 32 bits, the returned value is only different past the 10 millionths decimal place.

```
INPUT
E = GA10to2(90,2,-100,100)
D = GA2to10(E,2,-100,100)
E = GA10to2(90,16,-100,100);
D = GA2to10(E,16,-100,100)
OUTPUT
E =
     1     0
D =
   33.3333
D =
   89.9992
```

GA10to2 can also encode multiple values into a single binary string for simultaneous operation by the GA. This example is taken from the help text of the function, and will be returned to with the decoding function.

```
INPUT
E = GA10to2([0,0.63,1],[16,16,16],[-1,-1,-1],[1,1,1]);
disp([,'[',sprintf('%0.0f',E),']'])
OUTPUT
[011111111111111111010000101000111111111111111111]
```

9.7 Binary to Real Conversion

Syntax

real values = GA10to2(binary values, number bits, lower bounds, upper bounds);

Description

Convert a binary vector possibly encoding multiple real values back into a vector of real values. The binary vector should have been created by GA10to2.

Input / Output

- binary values - $(1 \times sum(\text{number bits}))$ vector holding p real values encoded as binary.
- number bits - $(1 \times p)$ vector with number of bits used to encode each real value.
- lower bounds - $(1 \times p)$ vector with lower bound of range for each real value.
- upper bounds - $(1 \times p)$ vector with upper bound of range for each real value.
- real values - $(1 \times p)$ vector of each decoded real value.

Algorithm

The first step taken by this decoding scheme is to separate the binary string S into separate strings - one for each encoded real value. Then, for each element, the real value is decoded using the formula in *equation 9.8*. As before, L and U represent the allowable range used for encoding, and B is the number of bits used.

$$R = L + \frac{(U-L)\sum_{i=0}^{B-1} S(i+1)\, 2^i}{\sum_{i=0}^{B-1} 2^i} \tag{9.8}$$

Example

Here we continue the example begin with GA10to2, and decode the binary string created. As you can see, GA2to10 correctly decoded the binary string.

```
INPUT
R = [0,0.63,1];
L = [-1,-1,-1];
U = [1,1,1];
B = [16,16,16];
E = GA10to2([0,0.63,1],B,U,L);
D = GA2to10(E,B,U,L)
OUTPUT
D =
    0.0000    0.6300    1.0000
```

9.8 Generation Seeding

Syntax

parents = GAselect(fitness scores, objective, method)

Description

Use fitness scores to select chromosomes from a generation in preparation for mating to produce the following generation.

Input / Output

- fitness scores - $(n \times 1)$ vector holding fitness score for each member of population. If n is not even, the score corresponding to the most fit chromosome will be inserted again.
- objective - Scalar indicating type of optimization: -1 = maximize, 1 = minimize.
- method - Scalar indicating pairing method: 1 = sorted, 2 = roulette.
- parents - $\left(\frac{n}{2} \times 2\right)$ matrix indicating pairs of solution indices to mate (by row).

Algorithm

For both generation seeding methods, the first step is to sort the current population by the objective function values, such that the ”most fit” chromosomes are at the beginning of the list. For the sorted method, no more preparation is necessary - the chromosomes are aligned for mating in sequential pairs ($mate(1,2)$, $mate(3,4)$, etc...).

The roulette method is akin to a biased roulette wheel, in which the individual bins are of varied size as in *Figure 9.3*. Bins for all chromosome are computed as $b_i = \left\{ \frac{2i}{n(n+1)} \mid b_i \in [0,1] \right\}$ (where $n =$ population size), then a cumulative sum of these bins is computed. As an example, consider the sorted list of 4 chromosomes - the bin widths are given as $b_i = \left[0.40\ 0.30\ 0.20\ 0.10\right]$, so the bin limits are as shown here.

bin	1	2	3	4
Lower Limit	0.00	0.40	0.70	0.90
Upper Limit	0.40	0.70	0.90	1.00

Clearly, the larger bins are at the beginning, corresponding to the most fit chromosomes. At this point, n random numbers are generated uniformly from $[0,1]$ and placed in the appropriate bin. For each random variate in bin i, chromosome i gets represented in the next generation. In this way, chromosomes with a better objective function value are overrepresented in the mating pool. The last step specific to this method is to randomly permute the ordering of the chromosomes. No matter which

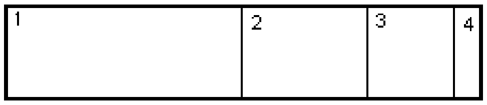


FIGURE 9.3: Conceptual roulette ”wheel”.

method is used, the final step is the same - reshape the vector of chromosome indices into the $\left(\frac{n}{2},2\right)$ parents matrix.

Example

```
INPUT
rand('state',1975)
fit = sort(rand(10,1),'descend');
S = GAselect(fit,-1,1);
R = GAselect(fit,-1,2);
disp(MatrixtoStr(fit))
disp(MatrixtoStr(S,'%02.0f'))
disp(MatrixtoStr(R,'%02.0f'))
S = GAselect(sort(rand(11,1),'descend'),1,1);
disp(MatrixtoStr(S,'%02.0f'))
OUTPUT
        1          1   2        1   2        1   2
  ----------    -------      -------      -------
 1| 0.75736| 1 |01 02|    1 |01 01|    1 |11 10|
 2| 0.74900| 2 |03 04|    2 |06 01|    2 |11 09|
 3| 0.70559| 3 |05 06|    3 |01 05|    3 |08 07|
 4| 0.65754| 4 |07 08|    4 |01 07|    4 |06 05|
 5| 0.60761| 5 |09 10|    5 |04 03|    5 |04 03|
 6| 0.53533|    -------      -------   6 |02 01|
 7| 0.51611|                              -------
 8| 0.27495|
 9| 0.16207|
10| 0.11422|
----------
```

Here we've already sorted the vector of fitness scores such that the most fit chromosomes (highest scores).are at the beginning of the vector. We can see that the sorted method (first output) seeds the next generation by simply pairing sequential chromosomes. The top two will be mated, as will the next two, with the sequence continuing through the entire population. However, in the second output, we see that the best solution will be mated 5 times! For the last computation, we've assumed a population of $n = 11$, and switch to a minimization GA - hence the best solutions are at the end of the vector. We see that the most fit chromosome was intelligently inserted into the parent vector, such that it will be mated with the 2nd and 3rd best individuals, and not with itself.

9.9 Chromosomal Crossover

Syntax

offspring = GAcrossover(population, parents, crossover rate, crossover type)

Description

Performs chromosomal crossover on the current generation of a GA after the solutions have been selected and paired for mating.

Input / Output

- population - $(n \times p)$ matrix of current GA population.
- parents - $\left(\frac{n}{2} \times 2\right)$ matrix indicating pairs of solution indices to mate from GAselect.
- crossover rate - Scalar probability of crossover in $[0,1]$.
- crossover type - Scalar indicating type of crossover to perform: 1 = single point, 2 = dual point, 3 = uniform.
- offspring - $(n \times p)$ matrix of next GA population.

Algorithm

There are three methods of crossover implemented by this function, and all three start by determining if a given mating pair will produce crossed-over or identical offspring. A random number is generated from the usual uniform distribution; if it is less than the probability of crossover, the parental chromosomes are crossed to form the offspring. Otherwise, they are merely duplicated unchanged.

single-point If single-point crossover is selected, an integer in $[1, p]$ is selected randomly. The parental chromosomes are then traded at this point such that the ”son” gets the $[1, X]$ portion of the ”dad’s” chromosome and the $[X+1, p]$ portion of the ”mom’s” chromosome. The ”daughter” binary string is the opposite.

dual-point In dual-point crossover, two crossover points are randomly selected, and the parent strings are divided into three portions: $[1, X_1]$, $[X_1+1, X_2]$, $[X_2+1, p]$. The son inherits the 1st and 3rd portions from the father and the 2nd from the mother. Again, the daughter is built out of what’s left.

uniform For the final method, p random uniform variates are generated, and those that are less than the crossover probability are trading points. The son is created by taking the points from the father corresponding to the trading points, with all others coming from the mother. The daughter is created in the reverse manner.

Table 9.4 has an example of each of these.

	Crossover Point(s)	Parents $\longrightarrow$Offspring
Single	2	$\begin{bmatrix}1\ 1\vert\ 1\ 1\ 1\ 1\\ 0\ 0\vert\ 0\ 0\ 0\ 0\end{bmatrix} \longrightarrow \begin{bmatrix}1\ 1\vert\ 0\ 0\ 0\ 0\\ 0\ 0\vert\ 1\ 1\ 1\ 1\end{bmatrix}$
Dual	$3,5$	$\begin{bmatrix}1\ 1\ 1\vert\ 1\ 1\vert\ 1\\ 0\ 0\ 0\vert\ 0\ 0\vert\ 0\end{bmatrix} \longrightarrow \begin{bmatrix}1\ 1\ 1\vert\ 0\ 0\vert\ 1\\ 0\ 0\ 0\vert\ 1\ 1\vert\ 0\end{bmatrix}$
Uniform	$1,3,5$	$\begin{bmatrix}1\vert\ 1\ 1\ 1\vert\ 1\vert\ 1\\ 0\vert\ 0\ 0\ 0\vert\ 0\vert\ 0\end{bmatrix} \longrightarrow \begin{bmatrix}1\vert\ 0\ 0\vert\ 1\ 1\vert\ 0\\ 0\vert\ 1\ 1\vert\ 0\ 0\vert\ 1\end{bmatrix}$

TABLE 9.4
Crossover Examples - ”|” Indicates Crossover Points

Example

In this example, we’ve taken the same population of just two individuals, and performed crossover using each of the three methods.

```
INPUT
rand('state',42)
P = [1,1,0,1,0;1,0,1,0,1];
S = GAcrossover(P,[1,2],1,1);
D = GAcrossover(P,[1,2],1,2);
```

```
U = GAcrossover(P,[1,2],0.8,3);
disp(MatrixtoStr(P,'%0.0f'))
disp(MatrixtoStr(S,'%0.0f'))
disp(MatrixtoStr(D,'%0.0f'))
disp(MatrixtoStr(U,'%0.0f'))
OUTPUT
   1 2 3 4 5
  -----------
1 |1  1  0  1  0|
2 |1  0  1  0  1|
  -----------
   1 2 3 4 5          1 2 3 4 5          1 2 3 4 5
  -----------        -----------        -----------
1 |1  1  1  0  1|   1 |1  0  1  1  0|   1 |1  1  0  1  1|
2 |1  0  0  1  0|   2 |1  1  0  0  1|   2 |1  0  1  0  0|
  -----------        -----------        -----------
```

Here we see that, for the single-point crossover method, $X = 2$ was chosen as the crossover point, while $X = [1,3]$ was chosen for the dual-point crossover. Finally, for the uniform method, the 2nd, 3rd, and 4th points were chosen.

9.10 Genetic Mutation

Syntax

mutated = GAmutation(population, mutation rate)

Description

Perform random mutation on a population of chromosomes, this is usually performed after a generation has mated and produced the next generation.

Input / Output

- population - $(n \times p)$ matrix of n offspring GA solutions.
- mutation rate - Scalar probability of mutation in $[0,1]$.
- mutated - $(n \times p)$ matrix of n mutated offspring GA solutions.

Algorithm

The algorithm for mutation is very simple. The first step is to generate an $(n \times p)$ matrix, M, of random numbers drawn from $U(0,1)$, using the Matlab rand function. Using the logical indexing capability of Matlab, any loci in the population that correspond to elements of M that are less than the mutation rate have their bits flipped - a *not* operation. This function is so simple, the code is shown here.

```
[num_chrom, p] = size(popul);
mutation_chances = mutat_rate > rand(num_chrom,p);
newpop = popul;
newpop(mutation_chances) = not(newpop(mutation_chances));
```

Example

We demonstrate how this function with a trivial example. First we create a GA population with $n = 100$ chromosomes all of length 100; however, all entries are 0. Using a mutation rate of 75%, we would expect approximately 7500 bits to be flipped; in this example, a close 7437 were.

```
INPUT
a = zeros(100,100);
mutat_rate = .75;
rand('state',42)
b = GAmutation(a,mutat_rate);
actual = sum(sum(b)
expect = prod(size(a))*mutat_rate
OUTPUT
actual =
        7437
expect =
        7500
```

Here we have a reasonably realistic example.

```
INPUT
rand('state',42)
GAmutation([0,1,1,0,1;0,1,0,0,1],0.10)
OUTPUT
ans =
     0     1     0     0     1
     0     1     0     0     1
```

9.11 GA Engineering

Syntax

new offspring = GAengineering(previous best, current best, current offspring, engineer rate)

Description

One criticism of the genetic algorithm is that, due to its stochastic nature, subsequent runs can end up with different solutions to the same problem. This is typically only a problem if a problem is very large and/or when the number of generations and population size parameters are set too low. One solution is to employ GA engineering. This function implements GA engineering, the point of which is to limit the variability between GA runs. It takes the best solution from the previous generation and the best solution from the current generation, and finds the difference. Where they are different, the bits from the previous best are inserted into the offspring of the current generation with the specified probability. This should only be called if the best from the previous generation is better than the current best.

Input / Output

- previous best - $(1 \times p)$ vector holding the chromosome of the best solution from the previous generation.
- current best - $(1 \times p)$ vector holding the chromosome of the best solution from the current generation.
- current offspring - $(n \times p)$ matrix of all offspring from the current generation.
- engineer rate - Scalar probability of engineering in $[0,1]$.
- new offspring - $(n \times p)$ matrix of all offspring from the current generation after being engineered.

Algorithm

The first step in GAengineering is to identify the differences between the best solutions of the previous and current generations, and their indices. Next, a vector of random probabilities is generated, having the same size as the next generation. Offspring corresponding with a random variate being less than the engineer rate have their bits at the difference indices set to the bit values of the previous generation best. For example, if the previous and current solutions are $\left[1\ 0\ 0\ 1\ 0\ 1\ 1\ 1\right]$ and $\left[1\ 0\ 1\ 1\ 0\ 0\ 1\ 0\right]$, respectively, and the previous best had a better score, the bits inserted into the next generation will be $\left[\_\ \_\ 0\ \_\ \_\ 1\ \_\ 1\right]$.

Example

Here we have an example with only three offspring. As can be seen below, the 1st and 2nd members of the next generation had $\left[\_\ \_\ 0\ \_\ \_\ 1\ \_\ 1\right]$ inserted into their chromosomes.

```
INPUT
pgbest = ([1,0,0,1,0,1,1,1] == 1);
cgbest = ([1,0,1,1,0,0,1,0] == 1);
cgoff = ([ones(1,8);zeros(1,8);...
   [ones(1,4),zeros(1,4)]] == 1);
rand('state',42)
engoff = GAengineering(pgbest, cgbest, cgoff, 0.5);
disp(MatrixtoStr(cgoff))
disp(MatrixtoStr(engoff))
OUTPUT
   1 2 3 4 5 6 7 8
  ----------------
1 |1 1 1 1 1 1 1 1|
2 |0 0 0 0 0 0 0 0|
3 |1 1 1 1 0 0 0 0|
  ----------------
   1 2 3 4 5 6 7 8
  ----------------
1 |1 1 0 1 1 1 1 1|
2 |0 0 0 0 0 1 0 1|
3 |1 1 1 1 0 0 0 0|
  ----------------
```

9.12 GA for Real-valued Function Optimization

Syntax

[best solution, best score] = GArealoptim(parameters, number bits, lower bounds, upper bounds, extra plot title, objective function, up to 5 parameters)

Description

This implements the genetic algorithm for optimization of real valued functions with p parameters. Binary representations, of length B_i for all p parameters are concatenated so that all GA operations are performed on a single binary string of length $\sum_{i=1}^{p} B_i$.

Input / Output

- parameters - (1×15) vector of GA parameters:
    1. population size - Number of chromosomes in each population.
    2. number generations - Maximum number of generations to perform.
    3. minimum number generations - Number of generations with insufficient improvement for early termination.
    4. convergence criteria - When testing for early termination, any improvement less than this is deemed to be none.
    5. elitism - Scalar indicating if the best chromosome cross generations unchanged: 1 = yes, 0 = no.
    6. generation seeding type - Scalar indicating generation seeding method to use, see GAselect.
    7. crossover rate - Scalar probability of crossover in $[0,1]$.
    8. crossover type - Scalar indicating type of crossover to perform, see GAcrossover.
    9. mutation rate - Scalar probability of mutation in $[0,1]$.
    10. GA engineering rate - Scalar probability of GA engineering in $[0,1]$.
    11. optimization goal - Scalar indicating which type of optimization to perform: 1 = maximization, -1 = minimization.
    12. progress plot flag - Scalar indicating when to update the GA progress plot: -1 = no plot, 1 = with each iteration, 0 = at end.
    13. 3d surface plot flag - Scalar indicating whether or not to create a 3-d surface plot of the objective function: 1 = yes, -1 = no. If elitism is on, this will be turned off.
    14. screen output flag - Scalar indicating what to print to the screen: -1 = nothing, 0 = summary only, 1 = summary and with each iteration.
    15. randomization - If 0 is passed, the random state will be set by sum(clock()*1000000), otherwise, the value passed is used as the state.
- number bits - $(1 \times p)$ vector with number of bits used to encode real values.
- lower bounds - $(1 \times p)$ vector with lower bound of range for real values.
- upper bounds - $(1 \times p)$ vector with upper bound of range for real values.
- extra title - String, extra information to put on plot titles (just [] if not desired).
- objective function - String indicating name of function to optimize
- P1 - Optional secondary parameter to pass objective function.
- P2 - Optional tertiary parameter to pass objective function.
- P3 - Optional fourth parameter to pass objective function.
- P4 - Optional fifth parameter to pass objective function.
- P5 - Optional sixth parameter to pass objective function.
- best solution - Scalar real value that optimized the objective function.
- best score - Scalar optimized value of objective function.

Example

Here we provide a simple example with the GA trying to find the maximum likelihood estimators $\hat{a}$ and $\hat{b}$ for the gamma distribution. We start by generating $n = 1000$ samples from *Gamma* $(2,3)$:

$$f(x) = \frac{1}{b^a \Gamma(a)} x^{a-1} e^{-ax^b}. \tag{9.9}$$

```
% simulate data
dist = 'GAM'; n = 1000;
reala = 2; realb = 3;
X = SimDistData(dist,n,[reala,realb],42);
% set up for GA
parms = [50,50,10,1e-5,1,2,0.75,1,0.10,0.50,1,0,-1,1,42];
[LB,UB] = EstParamRanges(dist,X);
% run GA
[maxloglike,mles] = GArealoptim(parms,[32;32],...
   LB,UB,dist,'ComputeLogLike',X,dist);
```

As can be seen below, the GA converged in 2.25 seconds to $\hat{\alpha} = 2.003$ and $\hat{b} = 2.992$. Given that these parameters are generally taken to be whole numbers, it's clear that this is equivalent to the true values of $a = 2$ and $b = 3$. From *Figure 9.4*, we see that the GA found this solution very quickly - by the 20th generation or so.

```
GA BEGAN
##################################################
Started on: 20071203_164209
Random State:        42
Maximum # Generations: 50
Minimum # of Generations: 10
Convergence Criteria: 1e-005
Population Size: 50
Crossover Rate: 0.75
Mutation Rate: 0.10
Crossover Method: SINGLE-POINT
Mating Method: ROULETTE
!!With Elitism ON, the probability of GA
   engineering has been set to 0.00!!
Elitism is: ON
Objective: MAXIMIZE
Objective Function: ComputeLogLike
##################################################
```

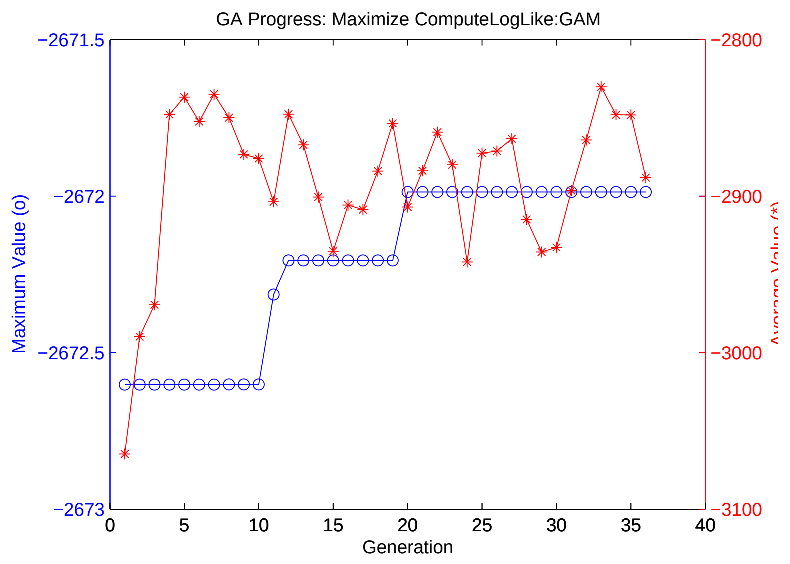


FIGURE 9.4: Sample GA Progress Plot.

```
Gen 1 of 50: Best = -2672.6021, Early Term = 1
Gen 3 of 50: Best = -2672.6021, Early Term = 3
Gen 5 of 50: Best = -2672.6021, Early Term = 5
...
Gen 31 of 50: Best = -2671.9865, Early Term = 5
Gen 33 of 50: Best = -2671.9865, Early Term = 7
Gen 35 of 50: Best = -2671.9865, Early Term = 9
Early Termination On Generation 36 of 50
Gen 36 of 50: Best = -2671.9865, Early Term = 10

====================================================
GA Complete
--------------------------------------
              ComputeLogLike Frequency
--------------------------------------
[2.003,2.992]    -2671.987       10
[2.003,2.992]    -2671.987       7
[1.963,3.057]    -2672.205       8
[1.963,3.022]    -2672.314       1
[1.947,3.031]    -2672.602       3
[1.947,3.031]    -2672.602       7
--------------------------------------
```

```
=====================================================
GA Completed in
    2.2500 Seconds
    0.0375 Minutes
    0.0006 Hours
```

9.13 GA Subsetting Template

Syntax

GAtemplate

Description

This is a general template used for creating and running the genetic algorithm for a variable subsetting problem.

Input / Output

All input is made by modifying the parameters for the GA in the section of the script with the % initialize model selection parameters comment heading.

- showtopsubs - Number of best subsets to show in the final summary.
- popul_size - Number of chromosomes in each population.
- num_generns - Maximum number of generations to perform.
- convgcrit - When testing for early termination, any improvement less than this is deemed to be none.
- elitism - Scalar indicating if the best chromosome cross generations unchanged: 1 = yes, 0 = no.
- sel_type - Scalar indicating generation seeding method to use, see GAselect.
- prob_xover - Scalar probability of crossover in $[0,1]$.
- xover_type - Scalar indicating type of crossover to perform, see GAcrossover.
- prob_mutate - Scalar probability of mutation in $[0,1]$.
- prob_engineer - Scalar probability of GA engineering in $[0,1]$.
- nochange_terminate - Number of generations with no improvement in objective to go before early termination.
- objec_func - String name of function to be optimized. The feval line in the code needs to be modified to pass parameters to this function correctly.

- maxmin - Scalar indicating which type of optimization to perform: 1 = maximization, -1 = minimization.
- pltflg - Scalar indicating when to update the GA progress plot: 1 = with each iteration, 0 = at end.
- plt3d - Scalar indicating whether or not to create a 3-d surface plot of the objective function: 1 = yes, 0 = no. If elitism is on, this will be turned off.
- randstate - If 0 is passed, the random state will be set by sum(clock()*1000000), otherwise, the value of randstate is used as the state.

No matter what values are entered for prob_engineer or plt3d, they will be set to 0.00 and 0, respectively, if the elitism rule is turned on. Output from GAtemplate is by way of up to four files saved in a "...\output \" directory.

- GASub_%objec_func%_%time started YYYYMMDD_HHMMSS%.mat - Matlab workspace file storing all parameters, data, and other relevant variables from a replication of the GA. The relevant variables include:
  - GA_BEST - A matrix holding the unique best results from all generations. The first column holds the fitness scores, the second has the number of generations that had that score as the best, and the rest of the columns are occupied by the solution chromosome associated with that score. The rows are sorted with the best results at the top.
  - allscores - A matrix storing all fitness scores for all generations - this is only created if the 3-d surface plot is.
  - save_prefix - A character string holding the identical prefix used for saving all the files.
  - ga_toc - The time in seconds required by the GA.
- GASub_%objec_func%_%time started YYYYMMDD_HHMMSS%.out - Text file storing GA progress and summary information printed into the Matlab command window.
- GASub_%objec_func%_%time started YYYYMMDD_HHMMSS%_GA.fig - Matlab figure file with GA progress plot showing the optimum score and average score from each generation.
- GASub_%objec_func%_%time started YYYYMMDD_HHMMSS%_3d.fig - Matlab figure file 3-dimensional surface plot of objective function - plotted with population on the X axis and generation on the Y axis (only created and saved if plt3d is on and elitism is off.

An obvious and well-asked question is why isn't the input through a GUI. This script was designed to be able to be run from a script that would perform multiple replications or a Monte Carlo experiment, with little modification. It wouldn't make sense to have to fill in some kind of GUI with the same data 1000 times! Additionally, while we could have also made it a function, rather than a script, we wanted to make a lot of variables available as output - it wouldn't make sense to have an output argument list with 20 or 30 items.

Algorithm

Variable subsetting is a statistical modeling problem that lends itself to the genetic algorithm very well. Consider some multivariate data $X \in \mathbb{R}^{n \times p}$, can we reduce the dimensionality of the data into q dimensions, with $q < p$? One context in which this is commonly a goal is regression - redundant covariates can have a negative effect on the least squares fit (see *Chapter 13 - Multivariate Regression*). If p is small, it is a simple manner to evaluate all possible subsets; for $p = 5$, for example, there are $2^5 - 1 = 31$ ways to combine the five variables. However, as p increases linearly, the number of possible subsets increases exponentially. Consider $p = 8$, there are 255 subsets models to evaluate. This where the GA can be a powerful tool. To cast the subsetting problem with $p = 8$ into the GA framework, consider a possible solution string $\begin{bmatrix}1 & 0 & 0 & 1 & 1 & 1 & 0 & 0\end{bmatrix}$ - if we use this for logical indexing of X in Matlab, the subset model includes variables $[1,4,5,6]$.

The GAtemplate script is an all-purpose GA implementation for this subsetting problem. Code can be inserted to do any data loading or preparation desired, and the objective function can be changed with only one real limitation. No matter how many out arguments it uses, the first must be the fitness score. Of course, with some coding, this can be bypassed. As written, this script can solve both maximization and minimization problems. GAtemplate follows the general GA flow as detailed in the introduction. Upon completion of the iterative procedure, the appropriate plots are created and saved and the best showtopsubs unique solutions and the associated scores from all generations are displayed in a table.

Example

We demonstrate this script with the familiar body fat dataset. This data is composed of body measurement observations from $n = 252$ men. There are $p = 13$ regressors, listed in *Table 9.5* - note that the two responses have been left off. Where not specified, measurements are in centimeters. We ran GAtemplate five times using the

x_1 =Age (yrs)	x_2 =Weight (lbs)
x_3 =Height (in)	x_4 =Neck circumference
x_5 =Chest circumference	x_6 =Abdomen 2 circumference
x_7 =Hip circumference	x_8 =Thigh circumference
x_9 =Knee circumference	x_{10} =Ankle circumference
x_{11} =Extended biceps circumference	x_{12} =Forearm circumference
x_{13} =Wrist circumference	

TABLE 9.5
Body fat dataset variables.

parameters shown here (from the final run).

```
##############################################
\output\GASub_MVGaussLogLike_20071128_095157
Started on: 20071128_095157
Random State: 2163062000
Maximum # Generations: 50
Minimum # of Generations: 30
Convergence Criteria: 0
Population Size: 30
Crossover Rate: 0.75
Mutation Rate: 0.10
Crossover Method: SINGLE-POINT
Mating Method: ROULETTE
GA Engineering Rate: 0.00
Elitism is: ON
Objective: MAXIMIZE
Objective Function: MVGaussLogLike
\data\BodyFatData.m
##############################################
```

There are a total of $2^{13} - 1 = 8191$ subsets; one run of the genetic algorithm will evaluate, unless it terminates early, at most $30 * 50 = 1500$ solutions. Recall that there is no artificial constraint to prevent the GA from reevaluating subsets. Thus, at most 18.3% of the subspace will be evaluated. As can be seen, the objective here is to find the subset that maximizes the multivariate Gaussian log likelihood. We are not claiming that this is a good model for this data. In fact, the tests for multivariate Gaussian kurtosis and skewness implemented in MVNormalityTest both strongly reject the null hypothesis of Gaussianity with p-values < 0.00000. Partial output from the final run is shown below, and the progress plot is shown in *Figure 9.5*.

```
==============================================
GA Complete
--------------------------------
     MVGaussLogLike Frequency
--------------------------------
{13}    -339.754        10
{12}    -534.339        24
{4}     -580.916        16
--------------------------------
==============================================
GA Completed in
    1.5780 Seconds
    0.0263 Minutes
    0.0004 Hours
```

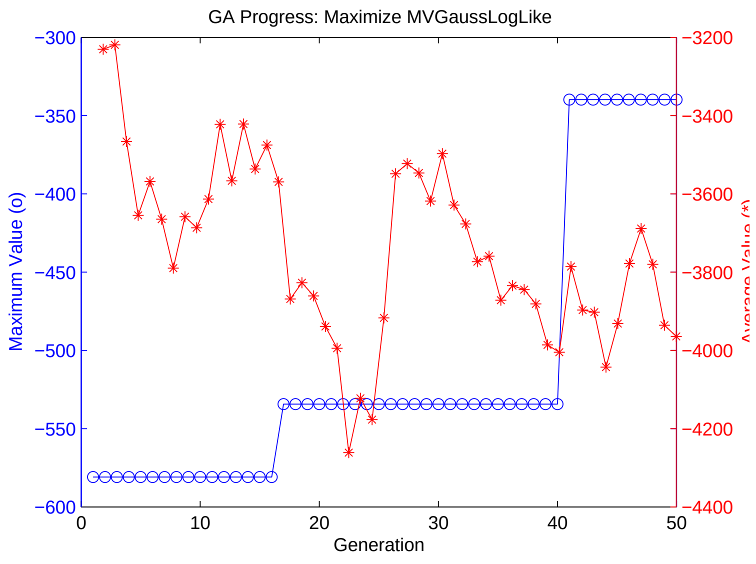


FIGURE 9.5: GA Progress Plot from Final Run.

These results were typical of all 5 runs - all selected the subset with only x_{13} = Wrist circumference. The same tests for normality applied to this subset were unable to reject the null hypothesis that the data came from a normal distribution, as seen in *Figure 9.6*. To show that this is actually a good solution, we wrote a second script, evalusubs_bodyfat, to compute the same objective function for all 8191 subsets of the body fat data and display the best 10. As can be see below, the GA honed in on the best subset; additionally, the other two solutions selected by any of the 50 generations were also in the top five. Thus we've demonstrated here that by only looking at 18.3% of the subset space (at most), the stochastic search performed as well as the much more computationally intensive all-subsets approach.

```
-----------------------
        MVGaussLogLike
-----------------------
{13}        -339.754
{10}        -490.033
{12}        -534.339
{9}         -578.927
```

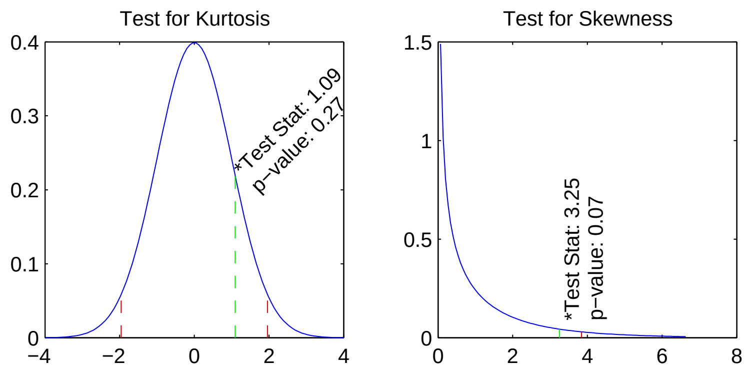


FIGURE 9.6: Normality Test Plots for Best Subset.

```
{4}         -580.916
{11}        -635.703
{3}         -684.230
{8}         -774.944
{10,13}     -782.087
{4,13}      -819.716
-----------------------
```

9.14 GA Parametric Model Estimation and Fitting

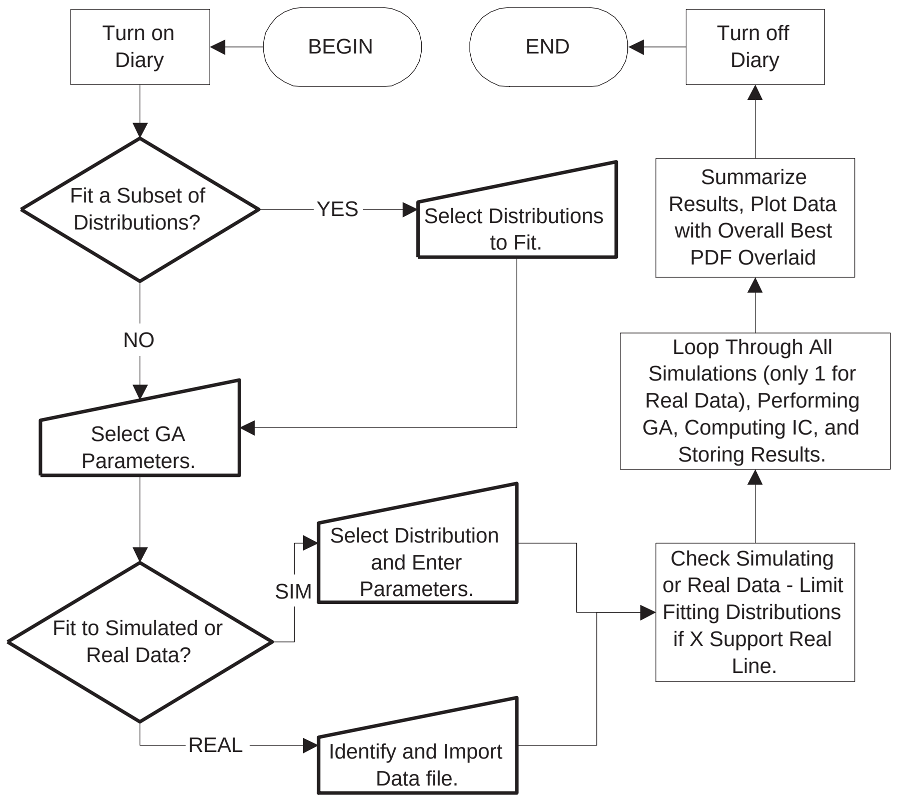
Syntax

drv_GAMLE

Description

Use the real-valued genetic algorithm to estimate parameters for various distributions fit to either simulated or real data, then use information criteria to pick the best model. This is a very flexible script, allowing the user to control the output, modify GA parameters, select the distribution (out of many) from which to simulate, and select a subset of distributions to fit.

Input / Output



Turn on Diary
BEGIN
END
Turn off Diary
Fit a Subset of Distributions?
YES
Select Distributions to Fit.
Summarize Results, Plot Data with Overall Best PDF Overlaid
NO
Loop Through All Simulations (only 1 for Real Data), Performing GA, Computing IC, and Storing Results.
Select GA Parameters.
Select Distribution and Enter Parameters.
SIM
Check Simulating or Real Data - Limit Fitting Distributions if X Support Real Line.
Fit to Simulated or Real Data?
REAL
Identify and Import Data file.

FIGURE 9.7: drv_GAMLE Flow Diagram.

The flow diagram in *Figure 9.7* identifies the sequence of activities in this script in general. Specifically of interest are the boxes with bold outlines. These are where the user provides input - either by a pop-up dialogue window, or through the command window. All of the parameters have been discussed elsewhere in this chapter, except for the Information Criteria (IC on flow). The current two choices are *AIC* and *SBC*, shown in *equations 9.11* and *9.10*, respectively.

All output is by way of screen output, which is saved into a Matlab diary file, and possibly several plots. Everything that is printed to the Matlab command window is saved into a human-readable text file named ”GAMLE_%time started YYYYMMDD_HHMMSS%”, saved in the directory in which the script resides. If the user has set the screen output flag to 0 or 1, this will include output from GArealoptim as appropriate. If either of the plotting flags (progress plot, surface plot) were not set to -1, these plots will be created - one per distribution fit per simulation. Be careful with the plotting flags, up to 11 distributions can be fit to data; for 10 simulations, that's 110 GA progress plots. Finally, a density histogram of the data - either the real data, or the final simulation - is constructed, and the overall best probability density function is overlaid.

Algorithm

For a parametric model, the two information criteria used by drv_GAMLE are shown below.

$$AIC = -2\log l\left(\hat{\theta} \mid X\right) + 2p \tag{9.10}$$

$$SBC = -2\log l\left(\hat{\theta} \mid X\right) + p\log n \tag{9.11}$$

Here, $\hat{\theta}$ indicates the maximum likelihood estimators determined by the GA, and p indicates the number of parameters estimated. You'll note on the flow diagram that one of the steps indicates the fitting distributions could be subset by the script. In the case of simulated data that could include negative values (such as $N(0,1)$), or real data that actually includes negative values, it doesn't make sense to fit strictly positive distributions, such as χ^2 to the data. drv_GAMLE figures this out by looking at the outputs returned by ComputeLogLike when no parameters are passed in.

One quirk that should be mentioned - GArealoptim knows nothing of the usual limitations on some distributional parameters, such as $\sigma > 0$ or $\nu \in \mathbb{N}$. Thus, it could very well optimize the Student's t with 3.65 degrees of freedom.

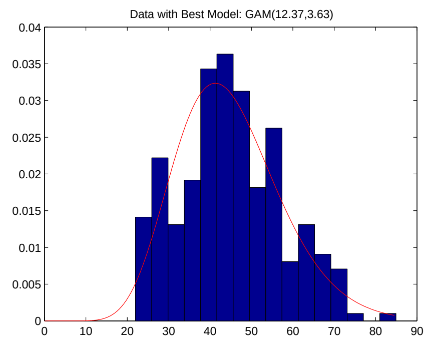
Example

We demonstrate this script using the first variable of the body fat data already used in this chapter - x_1 = age in years. The parameters used shown in the output below.

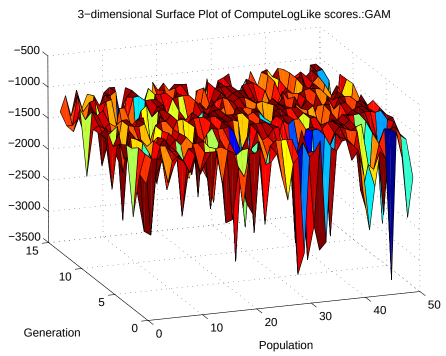
```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
drv_GAMLE began on 20071205_100557
----------------------------------------------------
NRM(mu,sigma): [45.02 12.87]: AIC = 1995.5015
GAM(a,b): [12.37 3.63]: AIC = 1989.5399
LOG(mu,sigma): [3.76 0.27]: AIC = 1997.7414
EXP(b): [44.82]: AIC = 2423.2678
WEI(a,b): [0.03 0.11]: AIC = 3724.7374
CHI(nu): [44.07]: AIC = 2042.6860
```

```
STU(nu): [0.22]: AIC = 3580.4350
CAU(theta): [43.30]: AIC = 2544.7308
LPL(mu,sigma): [43.33 5.12]: AIC = 2019.4872
PXP(mu,sigma,beta): [45.62 16.38 1.50]:
   AIC = 1996.0318
PAR(c): [0.26]: AIC = 3085.7170
BEST MODEL: GAM
----------------------------------------------------
====================================================
-GA Parameters-
Population Size: 50
Maximum # Generations: 50
Minimum # of Generations: 10
Convergence Criteria: 1e-005
Elitism is: OFF
Mating Method: ROULETTE
Mutation Rate: 0.10
Crossover Rate: 0.75
Crossover Method: SINGLE-POINT
GA Engineering Rate: 0.50
Randomizer:          0
Encoding Rate: 32
-Data Parameters-
Fit data in \data\BodyFatData.m
Number Observations: 252
====================================================
AIC Values
-----------------------------------------------
  NRM     GAM     LOG     EXP     WEI     CHI
-----------------------------------------------
1995.50 1989.54 1997.74 2423.27 3724.74 2042.69
-----------------------------------------------
-----------------------------------------
   STU   CAU     LPL     PXP     PAR
-----------------------------------------
 3580.43 2544.73 2019.49 1996.03 3085.72
------------------------------------------

Best Overall Model:
GAM(a,b): [12.37 3.63]: AIC = 1989.5399
Modeling Completed in
    14.1880 Seconds
    0.2365 Minutes
    0.0039 Hours
Diary file saved:GAMLE_20071205_100557.out
```



(9.8a) Data with Best Model



(9.8b) Likelihood Surface

FIGURE 9.8: Plots from Fitting Best Gamma Model to Body Fat Age Data.

@@

From the final summary, we see that the distribution that best fit this data was the gamma distribution, with the Gaussian distribution a close second choice. Of course, we'd probably round the parameters of the gamma distribution to $\hat{a} = 12$ and $\hat{b} = 3.5$, or something. Note that the script didn't even require a quarter of a minute to use the GA to optimize the fit of 11 distributions to the $n = 252$ observations. Here we show the histogram of the data with the best model overlaid, and the 3-d log likelihood surface plot of the best model.

9.15 Finding MLEs with Simulated Annealing

Syntax

[MLE, maximized likelihood] = SimAnneal_MLE(initial estimates, parameter limits, data, distribution, parameters)

Description

This implements an adaptive simulated annealing algorithm to find the maximum likelihood estimate(s) for the parameter(s) of certain distributional models.

Input / Output

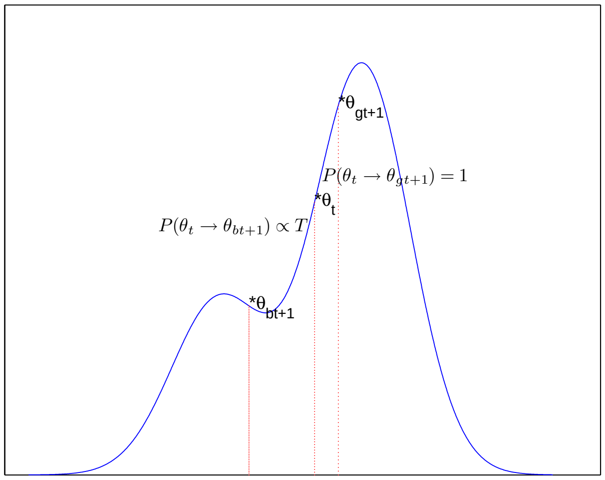
- initial estimates - $(1 \times p)$ vector of initial estimates for MLEs.
- parameters limits - $(1 \times p)$ vector describing limits on parameters:
  - -1 = none
  - 0 = nonnegative
  - 1 = strictly positive
- data - $(n \times 1)$ vector of data.
- distribution - Character code of distribution to use, from ComputeLogLike.
- parameters - (1×5) vector of parameters:
  1. beginning temperature (very problem dependent)
  2. maximum number of iterations
  3. randomization code: -1 = none, 0 = auto, else = pass in state
  4. screen output flag: 0 = no, 1 = yes
  5. progress plot flag: 0 = no, 1 = yes
- MLE - $(1 \times p)$ vector holding optimal parameter estimates.
- maximized likelihood - Scalar value of likelihood evaluated at MLE.

Algorithm

SimAnneal_MLE employs a temperature schedule such that the temperature in iteration k is $T_k = exp\left(-ck^{\frac{1}{p}}\right)$, where p is the dimension of the function space (number parameters estimated); we use $c = 1$. SA with this temperature schedule is called Adaptive Simulated Annealing (ASA). If a cooling schedule of $T_k = \frac{T_0}{k}$, is used, the process is called Cauchy Annealing. Boltzmann Annealing uses $T_k = \frac{T_0}{log(k)}$. Selection of T_0 is crucial to success of the procedure, as it is used in computing the probability with which the current state is moved to one with higher energy. If this ”bad” move was never allowed, the SA algorithm works just like a greedy algorithm. The way simulated annealing is designed, as the temperature decreases, the probability of making a bad move goes to 0. The idea is that when the temperature is high, we want to search enough of the state space so that as cooling occurs, we end up near a global optimum. *Figure 9.9* demonstrates how states evolve. If the energy of the current state, E_k, is less than the energy of the previous state, $E_(k-1)$, the algorithm moves to the current state. However, if $E_k > E_(k-1)$, a test value is computed as in *equation 9.12*.

$$exp(-fracE_k - E_(k-1)T_k) \tag{9.12}$$

If this test value is larger than a random variate drawn from $U\,(0,1)$, the algorithm moves to the current state. The question of how to generate neighboring states can be problem dependent. For our problem here, we’ve opted to generate neighbors based on a multivariate Gaussian distribution with $\Sigma = 2 * I_p$, centered at the state of the previous timestep.



*θgt+1
$P(\theta_t \to \theta_{gt+1}) = 1$
*θt
$P(\theta_t \to \theta_{bt+1}) \propto T$
*θbt+1

FIGURE 9.9: Simulated Annealing State Change Plot.

$$f(x_i \mid \mu, \Sigma) = (2\pi)^{-\frac{p}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x_i - \mu)' \Sigma^{-1} (x_i - \mu)\right) \tag{9.13}$$

Example

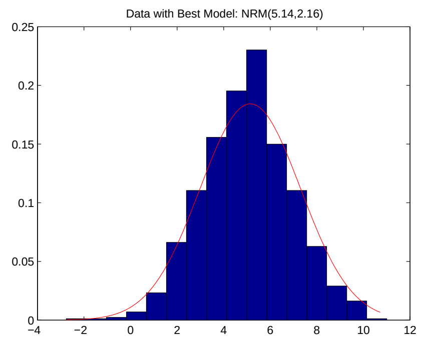
The script DemoSAMLE was written to demonstrate this function. It generates data from four distributions, and attempts to optimize their respective log likelihoods.

Distribution	Initial Values	Starting Temperature
$N(\mu = 5, \sigma = 2)$	$[-20, 0.25]$	100000
$\chi^2(\nu = 3)$	50	10000
$Gamma(a = 2, b = 0.5)$	$[5, 5]$	100000
$PE\left(\mu = -3, \sigma = 2, \beta = \frac{1}{2}\right)$	$[-2, 1.5, 0.25]$	100

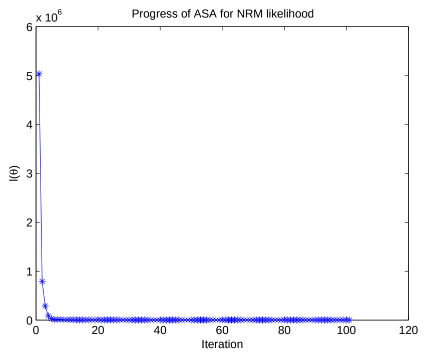
To it's credit, SA's dependence on the initial conditions, a problem in most gradient search methods, seems limited to the number of iterations required. However, the method does seem to be very dependent upon the initial temperature. The correct temperature seems to be related to both the dimension of the parameter space and the complexity of the problem. We also noted a strong effect of the stochastic nature of the algorithm. It's performance does not seems to be very consistent. With the exception of the power exponential distribution, ASA performed admirably. Partial screen output is shown below.

```
NORMAL
----------------
      mu  sigma
----------------   Maximized Log Likelihood at
True 5.00  2.00      True = -2068.249
MLE  5.14  2.16      MLE = -2082.210
----------------
CHI SQUARED
----------
      nu
----------   Maximized Log Likelihood at
True 3.00      True = -2093.888
MLE  3.08      MLE = -2094.284
----------
GAMMA
---------------
       a    b
---------------   Maximized Log Likelihood at
True 2.00 0.50      True = -884.650
MLE  1.66 0.58      MLE = -892.912
---------------
POWER EXPONENTIAL
----------------------
       mu  sigma beta
----------------------   Maximized Log Likelihood at
True -3.00  2.00 0.50      True = -3163.200
MLE  13.84 39.99 6.41      MLE = -4396.184
----------------------
```

Despite the very close starting values, and experiments with the initial temperature, we could not get the ASA function to end up with parameter estimates anywhere near the true values for the PE distribution. Selected plots are shown in *Figures 9.10* and *9.11*.

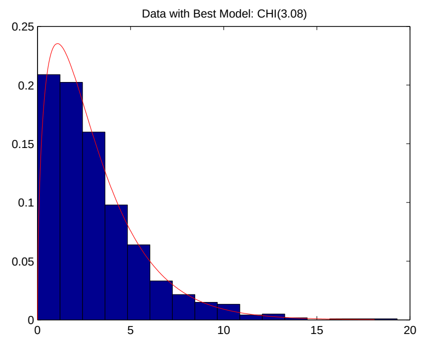


(9.10a) Data with Best Model

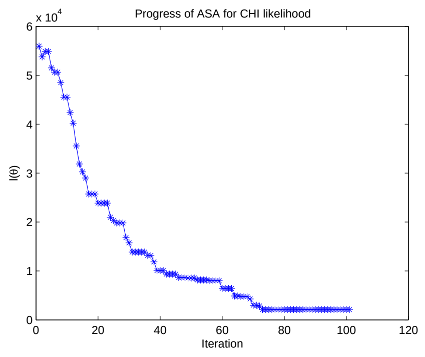


(9.10b) Likelihood Progress

FIGURE 9.10: Plots from Fitting Best Gaussian Model.



(9.11a) Data with Best Model



(9.11b) Likelihood Progress

FIGURE 9.11: Plots from Fitting Best χ^2 Model.