OPSEC v0.1 Manual

23 August 2011

This manual describes the usage of the OPSEC (Optimal Power Spectrum Estimation Code). The complete source code, as well as the latest version of this manual, are available at HOMEPAGE.

Contents

1	Formalism for Optimal Quadratic Estimators			
	1.1	Optimal mode functions	4	
	1.2	Examples	5	
	1.3	Derivation of optimal quadratic estimator	5	
	1.4	Optimality of quadratic estimator	7	
2	Imp	plementation Notes	7	
	2.1	Coordinate systems	7	
	2.2	Cell basis	7	
	2.3	Surveys	9	
	2.4	Models	9	
	2.5	Geometry of 2-point clustering	9	
3	Coc	le Details	10	

4	Bui	lding and running OPSEC	12
	3.8	Utility programs	12
	3.7	Configuration options for OPSEC programs	12
	3.6	Configuration files	12
	3.5	Annotated binary format	11
		3.4.5 estimate	11
		3.4.4 dot	11
		3.4.3 comma	11
		3.4.2 klt	11
		3.4.1 basis	10
	3.4	Programs	10
	3.3	Model class and subclasses	10
	3.2	Survey class and subclasses	10
	3.1	Cell structure	10

1 Formalism for Optimal Quadratic Estimators

OPSEC was designed primarily to measure the power spectrum of galaxies, specifically for the SDSS-III and SDSS-III catalogs of luminous red galaxies (LRGs). However, though several implementation choices were made with this measurement in mind, the formalism of optimal quadratic estimation that it follows is much more general. With the proper choice of inputs, OPSEC can be used to estimate any cosmological parameters from the clustering signal of any set of astrophysical objects. In this section we describe this broader formalism from a high-level, mathematical point of view. In later sections we specialize to the case of measuring P(k) from the large-scale clustering of galaxies.

To make use of OPSEC, three inputs must be given:

1. The observed number density field $n(\mathbf{r})$ for a particular tracer (equivalently, a list of positions $\{\mathbf{r}_g\}$).

- 2. The expected density $\bar{n}(\mathbf{r})$ of this tracer in the absence of clustering (usually estimated from the observed positions, taking into account the selection and masks used in the survey).
- 3. A model for how the observed 2-point correlation function depends on a set of cosmological parameters p_n ($1 \le n \le N_p$), along with a set of prior estimates $p_n^{(0)}$ for these parameters (usually from previous measurements).

These inputs are used to construct optimal estimates \hat{p}_n for the parameters p_n , as follows. (The precise sense in which these estimates are "optimal" is described in Section 1.4.)

First the observed density field $n(\mathbf{r})$ is collapsed into a set of real-valued coefficients y_i , by choosing a suitable set of mode functions $\psi_i(\mathbf{r})$, and defining

$$y_i = \int d^3r \ \psi_i(\mathbf{r})[n(\mathbf{r}) - \bar{n}(\mathbf{r})]. \tag{1}$$

(Here and in the following, 3-dimensional integrals are to extend only over the volume of the survey.) We refer to these coefficients y_i as "pixel values." The optimal choice of the mode functions ψ_i is itself a complicated issue, which we address in Section 1.1. For now, they may be viewed as an arbitrary set of N_m linearly independent functions defined over the survey volume. Regardless of the choice of mode functions, the pixel values y_i have zero mean: $\langle y_i \rangle = 0$.

Our tracers are presumed to be discrete objects (e.g. galaxies), and therefore their observed clustering pattern is subject to Poisson shot noise:

$$\langle n(\mathbf{r}_1)n(\mathbf{r}_2)\rangle = \bar{n}(\mathbf{r}_1)\bar{n}(\mathbf{r}_2)[1 + \xi(\mathbf{r}_1, \mathbf{r}_2)] + \bar{n}(\mathbf{r}_1)\delta_D(\mathbf{r}_2 - \mathbf{r}_1)$$
(2)

where δ_D is a Dirac delta function and $\xi(\mathbf{r}_1, \mathbf{r}_2)$ is the 2-point correlation function. The covariance of the pixel values can therefore be written as the sum of a signal component and a noise component,

$$\langle y_i y_i \rangle = C_{ii} = S_{ii} + N_{ii}, \tag{3}$$

where

$$S_{ij} = \int d^3r_1 \int d^3r_2 \ \psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2) \ \bar{n}(\boldsymbol{r}_1)\bar{n}(\boldsymbol{r}_2) \ \xi(\boldsymbol{r}_1,\boldsymbol{r}_2), \tag{4}$$

$$N_{ij} = \int d^3r \ \psi_i(\mathbf{r})\psi_j(\mathbf{r}) \ \bar{n}(\mathbf{r}). \tag{5}$$

We have defined the pixel values to have zero mean, since we are interested only in cosmological parameters that depend on the *clustering* of our tracers. Thus the lowest order statistics that can be meaningfully related to our parameters are quadratic combinations

$$\hat{p} = A_{ij} y_i y_j + b, \tag{6}$$

where summation over repeated indices is implied. We will frequently view A_{ij} as the components of a matrix, and y_i as components of a vector, and write $\hat{p} = \mathbf{y}^T \mathbf{A} \mathbf{y} + b$.

Under ideal circumstances (see Appendix 1.4 for details and caveats), it can be shown that the minimum variance, unbiased quadratic estimators for the parameters p_n are

$$\hat{p}_m = \sum_n (F^{-1})_{mn} (q_n - f_n) \tag{7}$$

where

$$q_n = \frac{1}{2} \mathbf{y}^T \mathbf{C}^{-1} \mathbf{C}_{,n} \mathbf{C}^{-1} \mathbf{y}, \tag{8}$$

$$f_n = \frac{1}{2} \operatorname{Tr} \left[\mathbf{C}^{-1} \mathbf{C}_{,n} \mathbf{C}^{-1} \mathbf{N} \right], \tag{9}$$

$$F_{mn} = \frac{1}{2} \operatorname{Tr} \left[\mathbf{C}^{-1} \mathbf{C}_{,m} \mathbf{C}^{-1} \mathbf{C}_{,n} \right], \tag{10}$$

and $\mathbf{C}_{,n}$ denotes the partial derivative $\partial \mathbf{C}/\partial p_n$. The matrices \mathbf{C} and $\mathbf{C}_{,n}$ here are to be evaluated at $p_n = p_n^{(0)}$, *i.e.* with the prior parameter estimates. F_{mn} is the Fisher matrix which, for minimum variance estimators, determines the error on \hat{p}_m ,

$$Cov[\hat{p}_m, \hat{p}_n] = (F^{-1})_{mn}.$$
 (11)

1.1 Optimal mode functions

The choice of the mode functions $\psi_i(r)$ affects the accuracy of the estimates \hat{p}_n . The optimal choice depends on the parameters that are to be estimated, the geometry of the survey, and the number density of the desired tracers. Following Tegmark *et. al.*, we choose the mode functions to be signal-to-noise eigenmodes. That is, we choose mode functions so that the signal and noise matrices (see Eqs. (4-5)) are simultaneously diagonal: $S_{ij} = s_i \delta_{ij}$ and $N_{ij} = n_i \delta_{ij}$ (no sum on *i*). Of the infinite number of possible mode functions, we choose a finite number N_m having the largest signal-to-noise eigenvalue $\lambda_i = s_i/n_i$.

More explicitly, these signal-to-noise eigenmodes are constructed through the following procedure. First, we choose a convenient basis of linearly independent functions $\{\varphi_a(\mathbf{r})\}$ defined over the survey geometry, and compute the signal and noise matrices in this basis,

$$\widehat{S}_{ab} = \int d^3r \int d^3r' \, \varphi_a(\mathbf{r}) \varphi_b(\mathbf{r}') \, \bar{n}(\mathbf{r}) \bar{n}(\mathbf{r}') \, \xi(\mathbf{r}, \mathbf{r}'), \tag{12}$$

$$\widehat{N}_{ab} = \int d^3r \ \varphi_a(\mathbf{r})\varphi_b(\mathbf{r}) \ \bar{n}(\mathbf{r}). \tag{13}$$

Next we solve the generalized eigenvalue problem

$$\widehat{\mathbf{S}}\mathbf{b} = \lambda \widehat{\mathbf{N}}\mathbf{b},\tag{14}$$

obtaining a complete set of eigenvectors $\{\mathbf{b}_i\}$ and associated eigenvalues $\{\lambda_i\}$. (This is possible since \widehat{S}_{ab} and \widehat{N}_{ab} are real symmetric matrices, and \widehat{N}_{ab} is positive-definite.) Then the functions

$$\psi_i(\mathbf{r}) = \sum_a b_{ia} \varphi_a(\mathbf{r}) \tag{15}$$

are signal-to-noise eigenmodes. For convenience, we normalize the ψ_i so that they are noise-orthonormal, *i.e.* so that the noise matrix is the identity: $N_{ij} = \delta_{ij}$. Then the covariance of pixel values in Eq. (3) becomes simply

$$\langle y_i y_j \rangle = C_{ij} = (1 + \lambda_i) \delta_{ij}$$
 (no sum on i). (16)

At this point, there are as many mode functions ψ_i as there are initial basis functions φ_a . However, many of these functions contribute very little information to the parameter estimates \hat{p}_n , in that the expectation of the quadratic combination y_i^2 is dominated by noise rather than the desired signal. Thus, by keeping only modes with the largest signal-to-noise eigenvalues λ_i , we can reduce the size of the computational problem without sacrificing too much information. In practice we first fix the desired number of modes N_m (the choice of which is informed by the desired error properties on our parameter estimates), then sort the eigenmodes by their signal-to-noise eigenvalue λ_i , and keep only the top N_m mode functions ψ_i .

This procedure is referred to by Tegmark et. al. as Karhunen-Loève compression. The mode functions ψ_i are then referred to as Karhunen-Loève mode functions, or simply KL modes.

1.2 Examples

1.3 Derivation of optimal quadratic estimator

Here we show how the quadratic estimator of Eq. (7) is derived. As our starting point, we note that the true covariance matrix of pixel values $C_{ij} = \langle y_i y_j \rangle$ is unknown. However, if our model is accurate and our prior estimates $p_n^{(0)}$ for the unknown parameter values p_n are close, then we can expand the true covariance matrix around our prior estimate for it,

$$C_{ij} = C_{ij}^{(0)} + \sum_{n=1}^{N_p} C_{ij,n}^{(0)}(p_n - p_n^{(0)}) + \dots,$$
(17)

where $\mathbf{C}^{(0)}$ and $\mathbf{C}_{,n}^{(0)}$ are the covariance matrix and its derivatives calculated using the prior estimates $p_n^{(0)}$. We have truncated the Taylor expansion at first order, which is a good approximation if the prior estimates $p_n^{(0)}$ are close to the true values p_n . (In fact, if \mathbf{C} depends linearly on the p_n , this expansion is exact.)

We want to construct estimators

$$\hat{p}_m = A_{mij} y_i y_j + b_m \tag{18}$$

that are unbiased, $\langle \hat{p}_m \rangle = p_m$, and for which the variance is minimized. (Throughout this section, summation is implied for repeated indices i, j, k, l, while sums over m or n are always written out

explicitly.) Given the above Taylor expansion for C_{ij} , we have

$$\langle \hat{p}_m \rangle = A_{mij} \sum_n C_{ij,n}^{(0)} p_n + A_{mij} \left[C_{ij}^{(0)} - \sum_n C_{ij,n}^{(0)} p_n^{(0)} \right] + b_m.$$
 (19)

So for \hat{p}_m to be unbiased, the coefficients A_{mij} must satisfy

$$A_{mij}C_{ij,n}^{(0)} = \operatorname{Tr}\left[\mathbf{A}_{m}\mathbf{C}_{,n}^{(0)}\right] = \delta_{mn},\tag{20}$$

while b_m is fixed to be

$$b_m = -A_{mij} \left[C_{ij}^{(0)} - \sum_n C_{ij,n}^{(0)} p_n^{(0)} \right] = -\operatorname{Tr} \left[\mathbf{A}_m \left(\mathbf{C}^{(0)} - \sum_n \mathbf{C}_{,n}^{(0)} p_n^{(0)} \right) \right]. \tag{21}$$

We now seek to minimize the variance

$$Var[\hat{p}_m] = A_{mij} A_{mkl} R_{ijkl} \tag{22}$$

where we have defined

$$R_{ijkl} = \langle y_i y_j y_k y_l \rangle - \langle y_i y_j \rangle \langle y_k y_l \rangle. \tag{23}$$

If we assume the pixel values y_i obey Gaussian statistics (see next section for more on this assumption), then

$$R_{ijkl} = C_{ik}C_{jl} + C_{il}C_{jk}. (24)$$

To minimize (22) subject to the constraint (20), we introduce Lagrange multipliers λ_n and define

$$S = A_{mij} A_{mkl} (C_{ik} C_{jl} + C_{il} C_{jk}) + \sum_{n} \lambda_n \left(A_{mij} C_{ij,n}^{(0)} - \delta_{mn} \right).$$
 (25)

Locating the extremum of this quantity yield the conditions

$$\frac{\partial S}{\partial A_{mij}} = A_{mkl} R_{ijkl} + \sum_{n} \lambda_n C_{ij,n}^{(0)} = 0, \tag{26}$$

$$\frac{\partial S}{\partial \lambda_n} = A_{mij} C_{ij,n}^{(0)} - \delta_{mn} = 0, \tag{27}$$

which admits the solution

$$\mathbf{A}_{m} = \sum_{n} (F^{-1})_{mn} \frac{1}{2} \mathbf{C}^{-1} \mathbf{C}_{,n}^{(0)} \mathbf{C}^{-1}, \tag{28}$$

where the Fisher matrix F_{mn} is given by Eq. (10).

(depends on true Cij, which is unknown...)

1.4 Optimality of quadratic estimator

- Discuss conditions under which estimator is optimal: priors and model are close to truth, and (ideally) signal matrix is linear in parameters.
- Show derivation using variance functional and Lagrange multipliers.
- Discuss choice of mixing matrix, explaining how M can help reduce correlations while only slightly increasing variance.

2 Implementation Notes

2.1 Coordinate systems

OPSEC supports two coordinate systems: spherical and Cartesian. In Cartesian coordinate mode, positions r are represented by a triple (x, y, z). In spherical coordinate mode, positions are represented by a triple (r, μ, φ) , where $\mu = \cos \theta$ is the cosine of the polar angle. The translation to or from Cartesian coordinates is given by

$$x = r\sqrt{1 - \mu^2}\cos\varphi, \qquad y = r\sqrt{1 - \mu^2}\sin\varphi, \qquad z = r\mu,$$
 (29)

$$r = \sqrt{x^2 + y^2 + z^2}, \qquad \mu = z/r, \qquad \varphi = \tan^{-1} y/x.$$
 (30)

2.2 Cell basis

As explained in Section 1.1, in order to compute the KL mode functions $\psi_i(\mathbf{r})$ we must first choose a basis of functions $\varphi_a(\mathbf{r})$ over the survey geometry. For OPSEC, we partition the survey geometry into a mesh of regularly-shaped cells, and choose our basis functions to be constant over each cell (i.e. $\varphi_a(\mathbf{r})$ is proportional to the indicator function over cell a). A detailed explanation is given below for the case of spherical coordinates; the Cartesian case is analogous.

First, a regular bounding region is defined, such that the entire survey fits within the region

$$\{(r,\mu,\varphi): \mathtt{RMin} \leq r \leq \mathtt{RMax}, \mathtt{MuMin} \leq \mu \leq \mathtt{MuMax}, \mathtt{PhiMin} \leq \varphi \leq \mathtt{PhiMax}\}. \tag{31}$$

This region is then subdivided into cells, by partitioning each coordinate interval into equal subintervals:

- [RMin, RMax] is divided into Nr equal subintervals $[r_d, r_{d+1}]$ for $0 \le d < \text{Nr}$.
- [MuMin, MuMax] is divided into Nmu equal subintervals $[\mu_e, \mu_{e+1}]$ for $0 \le e < \text{Nmu}$.
- [PhiMin, PhiMax] is divided into Nphi equal subintervals $[\varphi_f, \varphi_{f+1}]$ for $0 \le f < \text{Nphi}$.

(See Figure ??.) This subdivision of the bounding region gives a grid of Nr * Nmu * Nphi cells, each labeled by a triple (d, e, f):

$$C_{d,e,f} = [r_d, r_{d+1}] \times [\mu_e, \mu_{e+1}] \times [\varphi_f, \varphi_{f+1}]. \tag{32}$$

Note that, although each cell has the same thickness and the same angular extents,

$$\Delta r = \frac{\text{RMax} - \text{RMin}}{\text{Nr}}, \quad \Delta \mu = \frac{\text{MuMax} - \text{MuMin}}{\text{Nmu}}, \quad \Delta \varphi = \frac{\text{PhiMax} - \text{PhiMin}}{\text{Nphi}}, \quad (33)$$

their volumes will differ due to the varying radial positions:

$$V_{d,e,f} = \text{Vol } C_{d,e,f} = \frac{1}{3} (r_{d+1}^3 - r_d^3) \Delta \mu \Delta \varphi.$$
 (34)

(This is true only for the spherical case; for Cartesian coordinates all cells are identical.)

Most surveys are not regularly shaped, and consequently many of the cells in this grid will be wholly outside of the survey region. Rather than carrying these empty cells through our calculations, we discard them right away. Explicitly, we first order the cells within the grid by a grid index

$$G = (d * Nmu + e) * Nphi + f, \quad 0 \le G < Nr * Nmu * Nphi. \tag{35}$$

We then take all N_{cells} non-empty cells and label them by a consecutive index a, $0 \le a < N_{\text{cells}}$, according to the ordering imposed by G. Thus each non-empty cell can be labelled either by the cell index a, by the grid index G, or by the grid coordinates (d, e, f).

For each non-empty cell C_a we compute the number of galaxies expected to lie within the cell according to the given selection function,

$$\bar{N}_a = \int_{C_a} d^3 r \ \bar{n}(\mathbf{r}). \tag{36}$$

We also compute the effective volume of the cell, $V_{a,\text{eff}}$, which is defined as the volume of the cell for which $\bar{n}(\mathbf{r})$ is non-vanishing. (This isn't used for anything yet.)

For our basis functions, finally, we define

$$\varphi_a(\mathbf{r}) = \bar{N}_a^{-1/2} \chi_a(\mathbf{r}) = \begin{cases} \bar{N}_a^{-1/2} & \text{if } \mathbf{r} \in C_a, \\ 0 & \text{otherwise.} \end{cases}$$
(37)

The normalization factor $\bar{N}_a^{-1/2}$ is chosen so that the noise matrix is $\hat{N}_{ab} = \delta_{ab}$. The signal matrix in this basis is then given by

$$\widehat{S}_{ab} = \bar{N}_a^{-1/2} \bar{N}_b^{-1/2} \int_{C_a} d^3 r \int_{C_b} d^3 r' \ \bar{n}(\mathbf{r}) \bar{n}(\mathbf{r}') \ \xi(\mathbf{r}, \mathbf{r}')$$
(38)

$$\approx \bar{N}_a^{1/2} \bar{N}_b^{1/2} \int_{C_a} \frac{d^3 r}{V_a} \int_{C_b} \frac{d^3 r'}{V_b} \xi(\mathbf{r}, \mathbf{r}'). \tag{39}$$

The latter approximation is used in OPSEC as it leads to a significant optimization (see Appendix ??); it is a good approximation as long as the cells are small compared to the scale of density fluctuations we are trying to probe.

2.3 Surveys

[Describe Survey abstraction...]

2.4 Models

In Section 1, we mentioned that one of the inputs that OPSEC needs is a model for how the observed 2-point correlation function depends on the parameters p_n , as well as a set of prior estimates $p_n^{(0)}$. More precisely, OPSEC requires a prior estimate for the 2-point correlation function $\xi(\mathbf{r}_1, \mathbf{r}_2)$, as well as estimates for the functions $\xi_n(\mathbf{r}_1, \mathbf{r}_2)$, where as usual commas denote derivatives with respect parameters: $\xi_n = \partial \xi/\partial p_n$. These prior estimates are used in the construction of the matrices \mathbf{C} and \mathbf{C}_n in Eqs. (8), (9), and (10). Explicitly, the signal components of these matrices are given by

$$S_{ij} = \int d^3r_1 \int d^3r_2 \ \psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2) \ \bar{n}(\boldsymbol{r}_1)\bar{n}(\boldsymbol{r}_2) \ \xi(\boldsymbol{r}_1,\boldsymbol{r}_2), \tag{40}$$

$$S_{ij,n} = \int d^3r_1 \int d^3r_2 \ \psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2) \ \bar{n}(\boldsymbol{r}_1)\bar{n}(\boldsymbol{r}_2) \ \xi_{,n}(\boldsymbol{r}_1,\boldsymbol{r}_2). \tag{41}$$

The prior estimate for $\xi(\mathbf{r}_1, \mathbf{r}_2)$ is also used in the construction of the KL mode functions $\psi_i(\mathbf{r})$.

2.5 Geometry of 2-point clustering

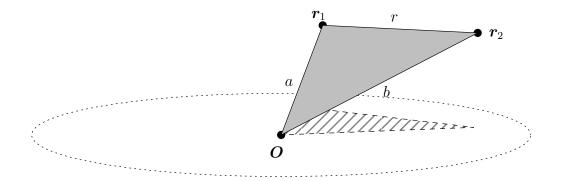
For a statistically isotropic field (which describes nearly every possible field in cosmology, including especially the redshift space galaxy number density), the 2-point correlation function $\xi(\mathbf{r}_1, \mathbf{r}_2)$ depends only on the geometry of the triangle formed by the observer \mathbf{O} and the two positions \mathbf{r}_1 , \mathbf{r}_2 .

Of the many possible ways of parameterizing this geometry, in OPSEC we use the three distances $r = |\mathbf{r}_2 - \mathbf{r}_1|$, $a = |\mathbf{r}_1 - \mathbf{O}|$, and $b = |\mathbf{r}_2 - \mathbf{O}|$ (see Figure ??). Thus, the correlation function and its derivatives are actually implemented as functions of these three scalars: $\xi(\mathbf{r}_1, \mathbf{r}_2) = \xi(r, a, b)$ and $\xi_{,n}(\mathbf{r}_1, \mathbf{r}_2) = \xi_{,n}(r, a, b)$.

3 Code Usage

3.1 Programs

The core functionality of OPSEC is broken into several independent programs. Each program performs a single logical operation, with well-defined input and output. Structuring the code in this way has a number of advantages:



- it's easier to develop, since each program performs a single task or a series of closely related tasks;
- it's easier to debug, since each program can be tested individually;
- it allows parts of the code to be re-run without having to completely restart the analysis (e.g. the same KL mode functions can be used for different model parameterizations).

In the following subsections we describe each program in more detail.

3.1.1 basis

The basis program is responsible for producing properly normalized basis functions $\varphi_a(r)$. For input it takes a specification of the survey, including its geometry and selection function, and for output it produces a list of non-empty cells (see Section 2.2). A cell is described by its cell index a, its coordinate bounds (min and max r, μ , and φ values in the spherical case), and the number of galaxies \bar{N}_a expected to lie within the cell.

3.1.2 klt

The klt program computes the signal-to-noise eigenvalues λ_i , and the corresponding eigenmodes $\psi_i(\mathbf{r})$ in terms of the basis functions $\varphi_a(\mathbf{r})$.

3.1.3 comma

The comma program computes the derivatives $C_{ij,n}$ of the covariance matrix with respect to parameters.

3.1.4 dot

The dot program computes the pixel values y_i using actual galaxy positions.

3.1.5 estimate

The estimate program performs the necessary linear algebra operations to obtain the minimum variance parameter estimates \hat{p}_m .

3.2 Annotated binary format

At various points in its operation OPSEC needs to store large, dense numerical arrays (vectors or matrices) on disk. A binary format is necessary both to minimize disk usage and to ensure fast reading and writing of the data. OPSEC uses annotated binary files, which generally carry a .abn suffix. A .abn file consists of a text header, followed by a special "tag" line describing the data, followed by the raw binary data itself. The text header can contain arbitrary text, which provides a convenient mechanism to document the origins and contents of the data. The tag line is of the form

where N indicates the number of data elements, SZ indicates the number of bytes per data element, E is a single character indicating whether the binary data is stored in little-endian (L) or big-endian (B) form, and FMT is a string that describes the intended type for the data elements. The format string follows the conventions of the Python struct module, described here: http://docs.python.org/library/struct.html#format-characters.

3.3 Configuration files

OPSEC is a fairly flexible system, and as such it needs to read in several parameter values so that it knows what to compute. It reads these values from simple ASCII configuration files, usually given a .cfg suffix. Each configuration file is a simple text file consisting of "name = value" pairs, where blank lines or lines beginning with the '#' character are ignored.

3.4 Configuration options for OPSEC programs

[List all required/accepted configuration options for each program, with a brief explanation of each.]

- 3.5 Utility programs
- 4 Code Details
- 5 Building and Running OPSEC