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Note on Blobel's Unfolding Method

1 Introduction and notation

The purpose of this note is to clarify the prescription used by Blobel [1] to determine the regularization parameter in unfolding. This involves a succession of transformations of variables such that the new variables have a diagonal covariance matrix. The procedure explained in [1] differs in certain respects from that implemented in the program `RUN` [2]; the algorithm of `RUN` is explained in Section 5.

The notation used here is that of *Statistical Data Analysis* [3]. The observed histogram $\mathbf{n} = (n_1, \ldots, n_N)$ is regarded as an N-dimensional random vector with expectation values $\boldsymbol{\nu} = E[\mathbf{n}]$. These are related to an M-dimensional "true" histogram $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_M)$ by

$$\boldsymbol{\nu} = R\boldsymbol{\mu} + \boldsymbol{\beta}, \tag{1}$$

where R is the response matrix and $\boldsymbol{\beta}$ is a vector of expected background values. Both R and $\boldsymbol{\beta}$ are assumed known.

The goal is to construct estimators $\hat{\boldsymbol{\mu}}$ for the true parameters $\boldsymbol{\mu}$. In regularized unfolding, these are found by minimizing

$$\begin{aligned} \Phi(\boldsymbol{\mu}) &= \chi^2(\boldsymbol{\mu}) + \tau \boldsymbol{\mu}^T G \boldsymbol{\mu} \\ &= (\mathbf{n} - \boldsymbol{\beta} - R\boldsymbol{\mu})^T V^{-1} (\mathbf{n} - \boldsymbol{\beta} - R\boldsymbol{\mu}) + \tau \boldsymbol{\mu}^T G \boldsymbol{\mu} \,. \end{aligned} \tag{2}$$

Here the covariance matrix of the data $V_{ij} = \mathrm{cov}[n_i, n_j]$ is assumed to be known and τ is the regularization parameter. The symmetric $M \times M$ matrix G can be chosen so that the regularization function function $\boldsymbol{\mu}^T G \boldsymbol{\mu}$ corresponds to the average curvature of the solution (see [1, 3]). Here, τ is attached to the regularization function rather than the log-likelihood, as done in [3].

2 The estimators $\hat{\boldsymbol{\mu}}$ for a given τ

For a given value of the regularization parameter τ, the estimators $\hat{\boldsymbol{\mu}}$ are found by setting the derivatives of Φ with respect to the μ_i equal to zero,

$$\nabla\Phi(\boldsymbol{\mu}) = -R^T V^{-1} (\mathbf{n} - \boldsymbol{\beta} - R\boldsymbol{\mu}) + \tau G \boldsymbol{\mu} = 0 \,. \tag{3}$$

The solution is

$$\hat{\boldsymbol{\mu}} = (R^T V^{-1} R + \tau G)^{-1} R^T V^{-1} (\mathbf{n} - \boldsymbol{\beta}) \equiv L(\mathbf{n} - \boldsymbol{\beta}) \,. \tag{4}$$

Since the estimators are linear functions of the data $\mathbf{n}$, the covariance matrix $U_{ij} = \mathrm{cov}[\hat{\mu}_i, \hat{\mu}_j]$ is found by error propagation to be

$$U = L V L^T \,. \tag{5}$$

If one considers the special case $\tau = 0$ (the unregularized solution), equation (4) reduces to $\hat{\boldsymbol{\mu}} = R^{-1}(\mathbf{n} - \boldsymbol{\beta})$; this solution will be denoted by $\hat{\boldsymbol{\mu}}_0$.

3 Transforming $\boldsymbol{\mu}$

Consider the function $\Phi(\boldsymbol{\mu})$,

$$
\begin{aligned}
\Phi(\boldsymbol{\mu}) &= (\mathbf{n} - \boldsymbol{\beta} - R\boldsymbol{\mu})^T V^{-1} (\mathbf{n} - \boldsymbol{\beta} - R\boldsymbol{\mu}) + \tau \boldsymbol{\mu}^T G \boldsymbol{\mu} \\
&= (\mathbf{n} - \boldsymbol{\beta})^T (\mathbf{n} - \boldsymbol{\beta}) - 2(\mathbf{n} - \boldsymbol{\beta})^T V^{-1} R\boldsymbol{\mu} + \boldsymbol{\mu}^T R^T V^{-1} R \boldsymbol{\mu} + \tau \boldsymbol{\mu}^T G \boldsymbol{\mu} ,
\end{aligned}
\tag{6}
$$

the minimum of which defines the regularized solution. In order to arrive at the prescription for determining τ, one must carrying out three transformations on $\boldsymbol{\mu}$. These are arranged such that the transformed quantities have a diagonal covariance matrix which reduces to the unit matrix for $\tau = 0$. The transformations are:

(1) an orthogonal transformation, $\mathbf{a} = A\boldsymbol{\mu}$, such that the quadratic term $\boldsymbol{\mu}^T R^T V^{-1} R \boldsymbol{\mu}$ in (6) takes on the form $\mathbf{a}^T B^2 \mathbf{a}$ with B^2 a diagonal matrix;

(2) a rescaling, $\mathbf{b} = B\mathbf{a}$, such that the quadratic term becomes $\mathbf{b}^T \mathbf{b}$, i.e. $B_{ii} = \sqrt{(B^2)_{ii}}$ and $B_{ij} = 0$ for $i \neq j$;

(3) an orthogonal transformation, $\mathbf{c} = C\mathbf{b}$, such that the regularization term in (6) can be expressed as $\tau \mathbf{c}^T D \mathbf{c}$ with D a diagonal matrix.

The columns of A are given by the eigenvectors of $R^T V^{-1} R$, the diagonal matrix B is defined by $B^2 = A R^T V^{-1} R A^T$, and the columns of C are given by the eigenvectors of $B^{-1} A G A^T B^{-1}$. Note that one has $\mathbf{b}^T \mathbf{b} = \mathbf{c}^T \mathbf{c}$, since the transformation $\mathbf{c} = C\mathbf{b}$ is orthogonal. The important ingredient here is the matrix D, which is given by

$$
D = C B^{-1} A G A^T B^{-1} C^T . \tag{7}
$$

After transforming to $\mathbf{c} = CBA\boldsymbol{\mu}$, equation (6) becomes

$$
\Phi(\mathbf{c}) = (\mathbf{n} - \boldsymbol{\beta})^T (\mathbf{n} - \boldsymbol{\beta}) - 2(\mathbf{n} - \boldsymbol{\beta})^T V^{-1} R A^T B^{-1} C^T \mathbf{c} + \mathbf{c}^T \mathbf{c} + \tau \mathbf{c}^T D \mathbf{c} . \tag{8}
$$

The solution is found by setting the derivatives of Φ with respect to c_i equal to zero,

$$
\nabla \Phi(\mathbf{c}) = -2 C B^{-1} A R^T V^{-1} (\mathbf{n} - \boldsymbol{\beta}) + 2\mathbf{c} + 2\tau D \mathbf{c} = 0 . \tag{9}
$$

This gives

$$
\begin{aligned}
\hat{\mathbf{c}} &= (1 + \tau D)^{-1} C B^{-1} A R^T V^{-1} (\mathbf{n} - \boldsymbol{\beta}) \\
&= (1 + \tau D)^{-1} \hat{\mathbf{c}}_0 .
\end{aligned}
\tag{10}
$$

where $\hat{\mathbf{c}}_0$ is the unregularized solution. The covariance matrix $W_{ij} = \mathrm{cov}[\hat{c}_i, \hat{c}_j]$ reduces to the simple diagonal form

$$
\begin{aligned}
W &= \left[(1 + \tau D)^{-1} C B^{-1} A R^T V^{-1} \right] V \left[(1 + \tau D)^{-1} C B^{-1} A R^T V^{-1} \right]^T \\
&= (1 + \tau D)^{-2} .
\end{aligned}
\tag{11}
$$

Note that the components of $\hat{\mathbf{c}}$ are uncorrelated, since D, and hence also W, is diagonal, and that in particular one has $W = 1$ for the unregularized solution ($\tau = 0$). The standard deviation of the ith component $\hat{c}_i$ is

$$
\sqrt{W_{ii}} = \frac{1}{1 + \tau D_{ii}} . \tag{12}
$$

4 The number of statistically significant components M_0 and the rule for determining τ

In order to formulate the rule for determining τ, one first needs to introduce the concept of the number of statistically significant components of the unregularized solution. The covariance matrix of $\hat{\mathbf{c}}_0$ is the unit matrix. Therefore, the value of each component $\hat{c}_{0i}$ tells how many standard deviations it is from zero. In [1] Blobel recommends a 95% confidence level corresponding to 1.96 standard deviations. Out of the M components, the number which satisfy

$$|\hat{c}_{0i}| \geq 1.96 \tag{13}$$

is called the number of statistically significant components, M_0.

For the unregularized estimators $\hat{\mathbf{c}}_0$, the sum of the absolute values of the standard deviations gives the number of components M. The idea for determining τ for the regularized solution is to make the corresponding sum equal to the number of statistically significant components M_0. That is, τ is defined by the relation

$$M_0 = \sum_{i=1}^{M} \sqrt{W_{ii}} = \sum_{i=1}^{M} \frac{1}{1+\tau D_{ii}} . \tag{14}$$

5 Implementation in RUN

The algorithm actually implemented in the most recent version of Blobel's program `RUN` [2] is somewhat different from that described above. First, the user is given the option to set by hand the number of statistically significant components M_0 by means of the input keyword `NRDF`, which sets the variable `NDF`. If this is set to zero, then the program uses a default algorithm to determine M_0, which is, however, different from the algorithm described in the previous section.

If `NDF` is input as zero, then the program first determines a provisional value of τ by solving

$$\begin{aligned} 0 &= \sum_{i=1}^{M} \left[(\hat{c}_{i0}^2 - \hat{c}_i^2) - 1 \right] \frac{3}{3+\tau D_{ii}} \\ &= \sum_{i=1}^{M} \left[\frac{\hat{c}_{i0}^2 (2\tau D_{ii} + \tau^2 D_{ii}^2)}{(1+\tau D_{ii})^2} - 1 \right] \frac{3}{3+\tau D_{ii}} . \end{aligned} \tag{15}$$

This is done in the routine `RSOLRT`. According to the comments in the routine, the idea is that the difference $\hat{c}_{i0}^2 - \hat{c}_i^2$ can be considered as the random noise, which should be one per bin. The terms are weighted by the factor $3/(3+\tau D_{ii})$ in order to suppress larger amplitudes.

This value of τ is then used to compute a provisional (non-integer) number of degrees of freedom (called `XDFR` in `RSOLRT`),

$$x_0 = \sum_{i=1}^{M} \frac{1}{1+\tau D_{ii}} \tag{16}$$

This is incremented by one and rounded down to the nearest integer to give M_0, which is then passed to the routine `RSOLEQ`. There, a new value of τ is determined according to equation (14), as described in the previous section. The statistical test for determining M_0 described in the previous section is not used.

One feature of the program as it stands is that the user may only choose an integer value for M_0, which leads to a discrete number of choices for τ. One way to bypass this is insert something like

```
if ( set_tau ) then
  tau = user_tau
  goto 20
endif
```

in the beginning of the routine `RSOLEQ`. The logical variable `set_tau` must be set equal to `.true.`, and the real variable `user_tau` set equal to whatever the user wants. These can be brought into `RSOLEQ` via a common block. For a starting value of τ, the default suggested by `RUN` can be used. This procedure seems to work except for extreme cases where one requests a very small τ; here the program apparently recognizes this as an abnormal condition and returns a much smoother solution than it should. Reasonable variations of τ about its preferred value seem, however, to work.

Another way of allowing for an adjustment of τ would be to modify equation (15) to be

$$0 = \sum_{i=1}^{M} \left[(\hat{c}_{i0}^2 - \hat{c}_i^2) - \gamma \right] \frac{3}{3 + \tau D_{ii}} . \tag{17}$$

By adjusting γ higher or lower than its default value of unity, the average amount random noise $\hat{c}_{i0}^2 - \hat{c}_i^2$ can be varied. This will result in a different value of x_0; if this changes by enough to change M_0 then a different τ will result.

References

[1] V. Blobel, Unfolding methods in high energy physics experiments, DESY 84-118 (1984); also in *Proceedings of the 1984 CERN School of Computing*, CERN 85-09 (1985).

[2] V. Blobel, The RUN manual: regularized unfolding for high-energy physics experiments, OPAL Technical Note TN361, March 8, 1996.

[3] G. Cowan, *Statistical Data Analysis*, Clarendon Press, Oxford (1998).