# INCLUSIVE VERTEXING

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### Abstract

The method of inclusive vertexing is based on a likelihood fit and allows to determine an arbitrary number of vertices for a set of measured tracks. The likelihood function is the probability that the tracks are produced at a given number of vertices. The fit returns the vertex positions and for each track relative probabilities that a track belongs to one of the vertices. The goodness of the fit is expressed in a quality factor. Additional quality factors for each track provides the possibility to find tracks which are unlikely to be produced at any of the vertices. The performance has been studied for B vertexing, where a B, a D and a main vertex were fitted in event hemispheres.

### 1 Introduction

Vertexing is solved by testing a vertex hypothesis and estimating the vertex positions. This is a two step procedure.

- 1. A hypothesis is formulated. E.g., a set of tracks originates from a common vertex and the tracks are distributed around the vertex according to a likelihood function  $\mathcal{L}$ .
- 2. (a) The free parameters (vertex positions,...) in  $\mathcal{L}$  are estimated by minimizing  $\mathcal{L} \to \mathcal{L}_{min}$ .
  - (b) The hypothesis can be disproved by calculating the probability  $\mathcal{P}$  to obtain a value  $\mathcal{L}$  which is smaller than  $\mathcal{L}_{min}$ :  $\mathcal{P} = \int_{<\mathcal{L}_{min}} d\mathcal{L}$ .

The usual method, exclusive vertexing, assigns tracks to vertices. The hypotheses are that subsets of tracks in an event originate from common vertices. This leads to more than one hypotheses per event which is the reason for two problems:

- The method can become unpractical due to limitations in computation time.
- If vertices are not well separated one can get more than one track combination with a reasonable probability. The wrong track combinations will lead to wrong (meaningless) estimations of vertex positions and wrong errors. This is always true if tracks exist which fit to more than one vertex, either because the vertices are too close together, a track is poorly measured or due to a large boost.

Exclusive vertexing is useful for particle reconstruction, where the additional information on the mass helps to suppress the background or allows to determine the amount of correct combinations on a statistical basis from a fit to the mass distribution.

This paper describes the method of inclusive vertexing where tracks are not assigned to vertices. The method works in a similar way as an unbinned maximum likelihood fit to a mass distribution. Suppose there are mass measurements  $m_i$  with a constant error  $\sigma_m$ . Finding the mass of two zero width resonances is a similar problem as to find the position of vertices. The mass measurements correspond to the space position measurements of tracks and the vertex position to the mass of a resonance. The number of resonance decays is the equivalent to the number of tracks produced at a vertex. Applying the method of exclusive vertexing to the mass measurement would mean to assign the measurements to one of the resonance and to perform one fit for each resonance. For each of these combinations one gets masses of the resonances and a probability for the fit. From all these combinations one then has to decide (on the basis of the fit probability) which fit result to choose. This is a nasty way to do a mass measurement and especially if the masses of the resonances are close together this will result in a bias and in wrong errors. The normal way to estimate the masses of the resonances doesn't assign single measurements to one of the resonances. One can never be sure to which resonance a measurement belongs. Therefore a likelihood is defined which is the sum of two gaussians and an unbinned maximum likelihood fit is performed. The method of inclusive vertexing uses this technique. Only one hypothesis will be made per event and a likelihood will be defined for this hypothesis. The minimization leads to the position of the vertices and the number of tracks produced at each vertex. In addition relative probabilities can be given for each track and vertex that the track is produced at this vertex. Advantages of this method are:

- There is no combinatorial problem and the computation time is approximately proportional to the number of tracks.
- There is only one result per event.
- Correlations between vertices can be included in the definition of the likelihood function.

The likelihood function will be defined in the next section, followed by a description of the minimization procedure and the determination of the goodness of the fit. The last section summarizes results of a performance test for  $Z^0 \to b\bar{b}$  decays.

#### The likelihood function 2

This section defines the likelihood function for the  $N^t$  measured tracks with parameters:

 $ec{r_i}^0 \ ec{r_i}^t \ V_i^t$ a vector pointing on the track i

a unit vector parallel to the track momentum

the track covariance matrix for the plane perpendicular to the track

direction

the momentum of track i  $p_i$ 

The hypothesis for the likelihood function is that the tracks are produced at  $N^{\nu}$ vertices. The free parameter in the likelihood  $\mathcal{L}(n_{\mu}, \vec{r}_{\mu})$  are the vertex positions  $\vec{r}_{\mu}$ and the number of tracks  $n_{\mu}$ , originating from vertex  $\mu$ . To construct the likelihood two approximations were made:

- Tracks have no curvature.
- There is no correlation between tracks. The likelihood is a product of probabilities for each track.

The likelihood

$$\mathcal{L}^t = \prod_i \mathcal{P}_i^t \cdot e^{-\mathcal{N}} \tag{1}$$

is based on a track probability density  $\mathcal{P}_i^t$ . The total number of tracks  $\mathcal{N} \equiv \int dP_i^t$  is equal to  $\mathcal{N} = \sum_{\mu} n_{\mu}$ .

The probability  $\mathcal{P}_i^t$  is the sum over the probabilities  $\mathcal{P}_{i\mu}^v$  that track i is produced at the vertex  $\mu$ :

$$\mathcal{P}_i^t = \sum_{\mu} \mathcal{P}_{i\mu}^v \tag{2}$$

with

$$\mathcal{P}_{i\mu}^{v} = n_{\mu} w_{i\mu} \, \mathcal{P}_{i\mu}^{r} \, \mathcal{P}_{i\mu}^{p} \tag{3}$$

and

: The number of tracks from vertex  $\mu$ .  $n_{\mu}$ 

: An a priori probability that track i comes from vertex  $\mu$ . This factor  $w_{i\mu}$ allows to include additional information like lepton identification.

: the probability to measure for track i the impact parameter  $\vec{d}_{i\mu}$  $\mathcal{P}^{r}_{i\mu}(\vec{r}_{\mu})$ with respect to vertex  $\mu$ .

$$\mathcal{P}_{i\mu}^r(\vec{r}_{\mu}) = \sum_k f_k G_{i\mu k} \tag{4}$$

$$G_{i\mu k} = \frac{1}{2\pi\sqrt{|V_{ik}|}} \exp\left(-\frac{1}{2}\vec{d}_{i\mu}V_{ik}^{-1}\vec{d}_{i\mu}\right)$$
 (5)

The sum of gaussians allows a description of tails in the resolution  $(\sum_{k} f_{k} = 1).$ 

 $\mathcal{P}^p_{i\mu}(p_{\parallel},p_{\perp}^2)$ : Particles, decaying at a secondary vertex, are boosted. Consequently the track directions  $\vec{r_i}^t$  are correlated with the flight direction of the mother particle. The flight direction is given by the difference  $\Delta \vec{r}_{\mu} = \vec{r}_{\mu} - \vec{r}_{ori(\mu)}$ , where  $ori(\mu)$  is the production vertex of the particle decaying at vertex  $\mu$ . This correlation has to be taken into account by including the probability to observe a track with the direction  $\vec{r_i}^t$  with respect to  $\Delta \vec{r_\mu}$ . It is convenient to describe this by using the transverse and longitudinal momentum, allowing for the approximation  $\mathcal{P}^p(p_{||},p_{\perp}^2) = \mathcal{P}^{p_{\perp}}(p_{\perp}^2) \mathcal{P}^{p_{||}}(p_{||})$ . Then only the component for the longitudinal momentum depends on the momentum spectrum of the decaying particle. The  $p_{\perp}$  spectrum is invariant.

The effect of including  $\mathcal{P}^p_{i\mu}$  is that small  $p_{\perp}$  values are favored. This includes naturally the jet direction in the fit. This also means that neutral tracks without tracking information can be used for the fit since they carry information on  $\Delta \vec{r}_{\mu}$ .

#### Additional constraints 2.1

Three additional constraint for the vertices are included in the likelihood:

$$\mathcal{L} = \mathcal{L}^t \cdot \mathcal{L}^c \tag{6}$$

with

$$\mathcal{L}^{c} = \prod_{\mu}^{vertices} \mathcal{P}_{\mu}^{pos} \, \mathcal{P}_{\mu}^{life} \, \mathcal{P}_{\mu}^{dir} \tag{7}$$

The constraints are:

### Vertex position constraint

A measurement of a vertex position  $\vec{r}_{\mu}^{c}$  is included by using the probability

$$\mathcal{P}_{\mu}^{pos}(\vec{r}_{\mu}) = \frac{1}{(2\pi)^{1.5} \sqrt{|V_{\mu}^{c}|}} \exp\left(-\frac{1}{2} (\vec{r}_{\mu} - \vec{r}_{\mu}^{c}) V_{\mu}^{c}^{-1} (\vec{r}_{\mu} - \vec{r}_{\mu}^{c})\right)$$
(8)

Examples are the main vertex constraint or for a secondary vertex a reconstructed  $\phi \to K^+K^-$  decay which is assumed to come from a  $D_s$  mesons.

### • Decay length

$$\mathcal{P}_{\mu}^{life}(\Delta \vec{r}_{\mu}) = \frac{1}{x_{\mu}} e^{-\Delta \vec{r}_{\mu}/x_{\mu}} \tag{9}$$

This allows to add information about the lifetime of decaying particles.

### • Flight direction The probability

$$\mathcal{P}_{\mu}^{dir}(\Delta \vec{r}_{\mu}) = \frac{1}{2\pi\sigma_{\alpha}} \exp\left(-\frac{\alpha_{\mu}^{2}}{2\sigma_{\alpha}^{2}}\right)$$
 (10)

$$\cos \alpha_{\mu} = \frac{\Delta \vec{r}_{\mu} \cdot \vec{u}_{\mu}}{|\Delta \vec{r}_{\mu}|} \tag{11}$$

constraints the flight direction  $\Delta \vec{r}_{\mu}$  to the direction  $\vec{u}_{\mu}$ . This constraint can be used to include the information from the jet direction without the need to specify the momentum distribution  $\mathcal{P}_{i\mu}^{p}(p_{\parallel}, p_{\perp}^{2})$ .

#### 2.2 Correcting for the poisson error on the number of tracks

Minimizing the likelihood function will give estimates for the vertex positions and for the number of tracks produced at each vertex. Since an extended maximum likelihood method is used the error on the number of tracks will contain the poisson error. The total number of tracks will be always  $\mathcal{N} = N$  with an error  $\sigma_{\mathcal{N}} = \sqrt{N}$ . The contribution from the poisson error can be eliminated by a transformation

$$(n_1, n_2, ..., n_{N^v}, \vec{r_1}, ... \vec{r_{N^v}}) \longrightarrow (\mathcal{N}, n'_2, ..., n'_{N^v}, \vec{r_1}^{v'}, ... \vec{r_{N^v}})$$
(12)

$$\mathcal{N} = \sum_{i\mu} n_i \tag{13}$$

$$n'_{\mu \ge 2} = n_{\mu \ge 2} \tag{14}$$

$$n'_{\mu \geq 2} = n_{\mu \geq 2}$$
 (14)  
 $\vec{r}_{\mu}^{\ \nu'} = \vec{r}_{\mu}$  (15)

and adding a constraint to the likelihood:

$$\mathcal{L} \longrightarrow \mathcal{L}' = \mathcal{L} \exp{-\frac{(\mathcal{N} - N^t)^2}{\epsilon}}$$
 (16)

with  $\epsilon \to \infty$ . This constraint does not change the position of the minimum of the likelihood function but subtracts the poisson errors on the number of tracks. The relation between the inverse of the covariance matrix

$$V'_{ij}^{-1} = \frac{\partial^2 - \ln \mathcal{L}'}{\partial p'_i \partial p'_i} \tag{17}$$

and  $V_{ij}^{-1}$  can be derived by using

$$\frac{\partial}{\partial n'_{\mu \geq 2}} = \frac{\partial}{\partial n_{\mu \geq 2}} - \frac{\partial}{\partial n_1} \tag{18}$$

For  $i, j \geq 2$  this leads to:

$$V'_{ij}^{-1} = V_{ij}^{-1}$$
 (19)  
 $-V_{i1}^{-1}$  if  $i \le N^{v}$  (20)  
 $-V_{1j}^{-1}$  if  $j \le N^{v}$  (21)  
 $+V_{11}^{-1}$  if  $i, j \le N^{v}$  (22)

$$-V_{i1}^{-1} \qquad \qquad \text{if } i \le N^{v} \tag{20}$$

$$-V_{i1}^{-1} if i \le N^{v} (20) 
-V_{1j}^{-1} if j \le N^{v} (21)$$

$$+V_{11}^{-1}$$
 if  $i,j \leq N^v$  (22)

This is the covariance matrix without poisson error. The number of tracks from vertex 1 is just given by  $n_1 = N^t - \sum_{\mu \geq 2} n_{\mu}$ .

#### 2.3 Track classes

Usually tracks can be divided in hemispheres or jets. Only tracks from one hemisphere or jet can come from the same secondary vertex. This should be directly included in the likelihood to avoid problems with the definition of  $\mathcal{P}_{i\mu}^p$  and to save computation time. For this reason track classes are defined for each event. Each track belongs to exactly one track class. E.g., there can be one track class for each jet. Each vertex might belong to more than one vertex (every secondary vertex belongs to one jet while the main vertex belongs to all classes since all tracks could come from the main vertex). The track likelihood is replaced by a product of likelihoods for each class:

$$\mathcal{L}^t = \prod_{c}^{classes} \mathcal{L}_c^t \tag{23}$$

This increases the number of parameters  $n_{\mu}$ . There are now parameters for each class  $n_{\mu}^{c}$  where  $\mu$  stays for all vertices in class c. It is straight forward to generalize the formulas in this note for track classes.

#### **Minimization** 3

The log likelihood  $F \equiv -\ln \mathcal{L}$  is a function of  $N^p$  parameters  $\vec{p} = (n_1^c, n_2^c, ..., n_{N^c, v}^c, \vec{r_1}, ... \vec{r_{N^v}})$ . The minimization of the likelihood function is an iterative procedure beginning with

a start vector  $\vec{p_1}$ . At any step k in the minimization the next parameter vector  $\vec{p_{k+1}}$  is derived from  $\vec{p_k}$  by using a second order Taylor expansion

$$F(\vec{p}) = F(\vec{p}_k) + \vec{g}\Delta\vec{p} + \frac{1}{2}\Delta\vec{p}G\Delta\vec{p}$$
 (24)

with  $\Delta \vec{p} = \vec{p} - \vec{p_k}$ . The first and second order derivatives

$$\vec{g} = \frac{\partial - \ln \mathcal{L}}{\partial \vec{p}} \bigg|_{\vec{p}_{b}} \tag{25}$$

$$G = \frac{\partial^2 - \ln \mathcal{L}}{\partial \vec{p} \partial \vec{p}} \Big|_{\vec{p_k}}$$
 (26)

are explicitly given in the appendix.

If G is positive definite normal procedures like the Newton method can be used. This can not be guaranteed here. It is possible that no or one track is produced at a vertex. In this case the vertex position is not fully defined, if there are no other constraints. Directions in the parameter space, where the likelihood has no maximum can be determined by calculating the eigenvalues  $e_i$  and eigenvectors  $\vec{v}_i$  of G. If an eigenvalue is close to zero the corresponding eigenvector gives the direction which is not well constrained. This can be shown by using the eigenvectors as coordinates  $\Delta \vec{p} = \sum_i a_i \vec{v}_i$ . The  $N^p$  dimensional problem then splits in  $N^p$  one dimensional problems

$$F(\vec{a}) = F(\vec{a}) + \sum_{i} a_{i} g_{i} + \frac{1}{2} \sum_{i} a_{i}^{2} e_{i}$$
 (27)

with  $g_i = \vec{g}\vec{v}_i$ . The minimum of  $F(\vec{a})$  is at

$$a_i = -\frac{g_i}{e_i} \tag{28}$$

The directions  $\vec{v_i}$  can be treated separately. There is no minimum of F, if  $e_i \leq 0$ . This could be because the likelihood is not constraint in this direction or because the second order expansion is not a sufficient approximation for  $F(\vec{p})$ . One then has to search for a minimum along the corresponding direction of the eigenvector.

It is also convenient to use the eigenvalues to calculate the covariance matrix to avoid the inversion of G.

$$V_{ij} = \sum_{k} E_{ik} \frac{1}{e_k} E_{jk} \tag{29}$$

with

$$E = (\vec{v}_1, \vec{v}_2, ..., \vec{v}_{NP}) \tag{30}$$

# 4 Quality factors

From the minimization one obtains the likelihood  $\mathcal{L}_{min}$ . To test if the assumed likelihood function agrees with the data the probability to observe a smaller value for the likelihood  $\mathcal{L} < \mathcal{L}_{min}$ , assuming the parameters found by the minimization are

track position measurement	$Q_{i}^{t} = \min_{\mu} \sum_{k} f_{k} P(\vec{d}_{i\mu} V_{ik}^{-1} \vec{d}_{i\mu}, 2[1 - 3/N_{\mu}^{m}])$
vertex position constraint	$Q_{\mu}^{pos} = P([\vec{r}_{\mu} - \vec{r}_{\mu}^{t}]V_{\mu}^{-1}[\vec{r}_{\mu} - \vec{r}_{\mu}^{t}], 3[1 - 3/N_{\mu}^{m}])$
vertex direction	$Q_{\mu}^{dir} = P(\alpha_{\mu}^{2}/\sigma_{\alpha_{\mu}}^{2}, 2-1.5/N_{\mu}^{m} - 1.5/N_{cor(\mu)}^{m})$
vertex probability	$Q_{\mu} = P(\sum_{i} \chi_{i\mu}^{t} + \chi_{\mu}^{dir} + \chi_{\mu}^{pos} + \chi_{\mu}^{pos} + N_{\mu}^{m} - 3)$
overall quality	$Q = P(\sum_{\mu i} \chi^2, \sum_{\mu} N_{\mu}^m - 3 \cdot N^v)$

Table 1: Definition of quality factors

the true ones, can be calculated. For a gaussian distribution it is given by the  $\chi^2$  probability

$$Q = P(\chi^2, N_{DoF}) = \int_{\chi^2}^{\infty} \frac{2^{-N_{DoF}/2}}{\Gamma(N_{DoF}/2)} (\chi')^{N_{DoF}/2} e^{-\chi'^2/2} d\chi'^2$$
 (31)

which is the PROB function on CERNLIB. The degrees of freedom  $N_{DoF}$  is the dimension of the parameter space minus the number of free parameters in the likelihood. The likelihood function for the inclusive vertexing is too complicated to do the integration. Instead a quality factors Q will be defined by using the gaussian contributions to the likelihood (see table 1). The number used for the degrees of freedom takes into account the "number of measurements" for vertex  $\mu$ :  $N_{\mu}^{m} = 2 \cdot n_{\mu} + 3$  (for a constraint on the vertex position)+1 (for a constraint on the flight direction).

# 5 Program package VNFIT

# 5.1 Program Code

The main fit program VNFIT is stored with all subroutines on ALOHA in the library: /u3/xu/oest/vertexfit/vnfit0

The input for the fit (track parameters, number of vertices to be fitted,...) has to be passed to the fit by filling the input COMMON VNINPUT in /u3/xu/oest/vertexfit/vnfit0/vncomm.inc.

QVNHEM on /u3/xu/oest/vertexfit/alpha0 is an example for a B, D and main vertex fit for one hemisphere. To run QVNHEM on has to

- link the libraries
   /u3/xu/oest/vertexfit/alpha0/ligsaga.a (for OSF/1)
   /u3/xu/oest/vertexfit/alpha0/libshift.a (for IRIX)
   and
   /cern/nag/libnag.a
- specify the input variables for QVNHEM as explained in the routine.

The vertex information from the fit is stored in the output COMMON VNOUT in /u3/xu/oest/vertexfit/vnfit0/vncomm.inc.

```
• The number of tracks from the main vertex PAR(1) \equiv N^t-PAR(2)-PAR(3), 
B vertex PAR(2), 
D vertex PAR(3).
```

- The vertex positions x, y, z for the main vertex PAR(4),...,PAR(6),
  B vertex PAR(7),...,PAR(9),
  D vertex PAR(10),...,PAR(12).
- The covariance matrix DCOVAR(i,j) for PAR(1),...,PAR(12).

The output COMMON contains further fit information like the quality factors. The routine itself returns

```
DLI the difference in -log likelihood between the three vertex fit and the case of having only one main vertex.
```

XMV the B+D vertex mass. XCV the B+D vertex charge.

The program QVNHEM is not a final version and should be modified for different analysis. This concerns the track selection (ITRQUA, QADJET), the V0 selection (QVO, IVOQUA), the tails for the track resolution (QTRKPA, QVOPA), the momentum spectrum for tracks (VNLIPF) and the determination of start values for the fit (VNSTRT).

# 5.2 Hemisphere Fit

The program QVNHEM has been used to fit three vertices in 1993 HVFL04 Monte Carlo events. The hemispheres are defined by the thrust axis, requiring  $|\cos\vartheta_{thrust}| < 0.7$ . The likelihood contribution  $\mathcal{P}^p_{i\mu}(p_{||}, p_{\perp}^2)$  was not used in the fit (DL = .FALSE.). The results of the fit for a B tag and vertex charge reconstruction are displayed in figures 1,2 and figure 3, respectively.

### 6 Conclusion

The method of inclusive vertexing estimates vertex positions without assigning tracks to vertices. The program package VNFIT allows to fit an arbitrary number of vertices to a given set of tracks. The fit returns vertex positions, probabilities for each track to belong to one of the vertices and quality factors which describes the goodness of the fit. Additional information like lepton identification or different momentum spectra for particles from different vertices can be included in a consistent way. As an example a B fit with three vertices has been studied and found to work with a good performance.

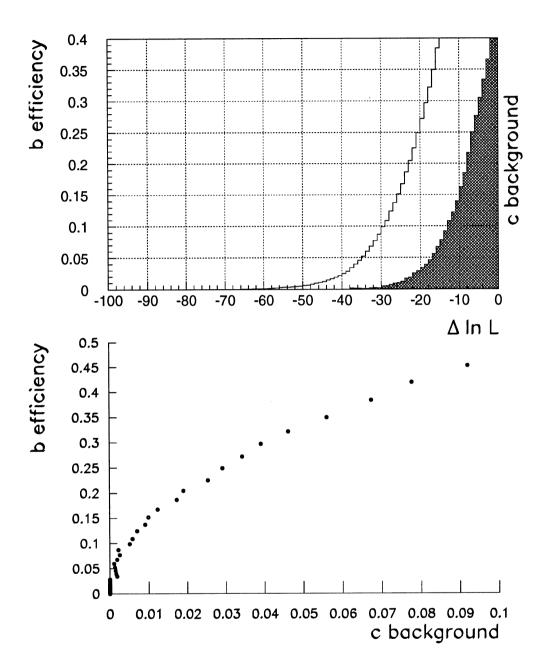


Figure 1: b reconstruction efficiency as a function of a cut on the difference in log likelihood (DLI) between the three vertex fit and the assumption of only one (main) vertex. The c background is shown as full histogram. The b efficiency versus c background which can be obtained is displayed below. Efficiencies are given for events with  $|\cos\vartheta_{thrust}| < 0.7$  and a event selection efficiency of 63.8% for  $b\bar{b}$  events.

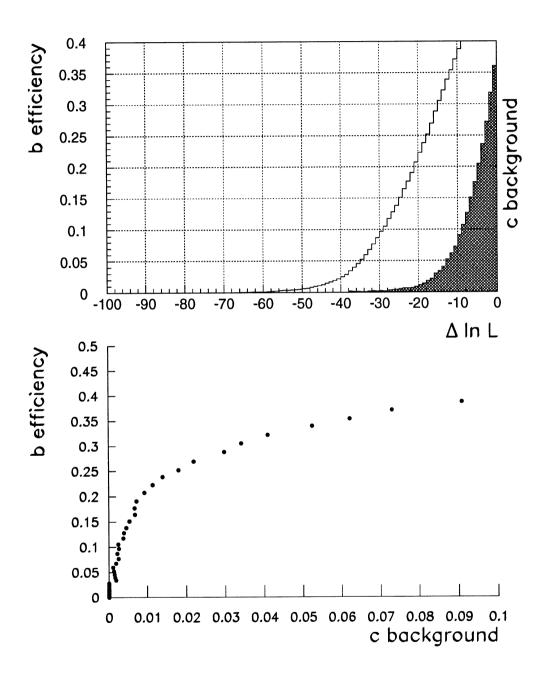


Figure 2: Same as figure 1 with a cut on the vertex mass 1.9 GeV <XMV< 5.5 GeV for DLI> -30.

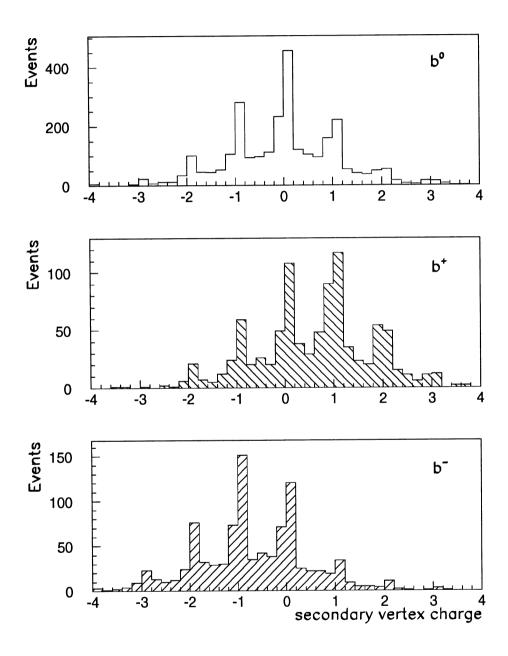


Figure 3: B+D vertex charge for events where both vertices are displaced from the main vertex by more than 0.5 mm.

## A Derivatives of $-\ln \mathcal{L}$

### A.1 Likelihood definition

$$\mathcal{L} = \mathcal{L}^t \mathcal{L}^c \tag{32}$$

$$\mathcal{L}_{t} = \prod_{i} \mathcal{P}_{i}^{t} \cdot e^{-\mathcal{N}}$$
 (33)

$$-\ln \mathcal{L}^t = \sum_{i}^{i} -\ln \mathcal{P}_i^t + \mathcal{N}$$
 (34)

$$\mathcal{N} = \sum_{\mu} n_{\mu} \tag{35}$$

$$\mathcal{P}_{i}^{t} = \sum_{\mu} \mathcal{P}_{i\mu}^{v} \tag{36}$$

$$\mathcal{P}_{i\mu}^{v} = n_{\mu}w_{i\mu} \mathcal{P}_{i\mu}^{r} \mathcal{P}_{i\mu}^{p}(p, p_{\perp}^{2}) \tag{37}$$

$$\mathcal{P}_{i\mu}^{r} = \sum_{k} f_{k} G_{i\mu k} \tag{38}$$

$$G_{i\mu k} = \frac{1}{2\pi\sqrt{|V_{ik}|}} \exp\left(-\frac{1}{2}\vec{d}_{i\mu}V_{ik}^{-1}\vec{d}_{i\mu}\right)$$
 (39)

$$\mathcal{R}_{i\mu k}^{r} = \frac{G_{i\mu k}}{\mathcal{P}_{i\mu}^{r}} \tag{40}$$

$$\mathcal{R}_{i\mu} = \frac{\mathcal{P}^{v}_{i\mu}}{\mathcal{P}^{t}_{i}} \tag{41}$$

# A.2 First and second order derivatives of $-\ln \mathcal{L}^t$

$$\frac{\partial - \ln \mathcal{L}^t}{\partial n_{\mu}} = \sum_{i} w_{i\mu} + \sum_{i} \frac{\partial - \ln \mathcal{P}_i^t}{\partial n_{\mu}}$$
(42)

$$\frac{\partial^2 - \ln \mathcal{L}^t}{\partial n_{\mu} \partial n_{\nu}} = \sum_{i} \frac{\partial^2 - \ln \mathcal{P}_i^t}{\partial n_{\mu} \partial n_{\nu}}$$
(43)

(44)

 $\frac{\partial - \ln \mathcal{P}_{i}^{t}}{\partial x} = 1 + \frac{\partial - \ln \mathcal{P}_{i\mu}^{v}}{\partial x} \tag{45}$ 

$$\frac{\partial^{2} - \ln \mathcal{P}_{i}^{t}}{\partial x \, \partial y} = \frac{\partial - \ln \mathcal{P}_{i}^{t}}{\partial x} \frac{\partial - \ln \mathcal{P}_{i}^{t}}{\partial y} + \tag{46}$$

$$\sum_{\mu} \mathcal{R}_{i\mu} \left( \frac{\partial^{2} - \ln \mathcal{P}_{i\mu}^{v}}{\partial x \partial y} - \frac{\partial - \ln \mathcal{P}_{i\mu}^{v}}{\partial x} \frac{\partial - \ln \mathcal{P}_{i\mu}^{v}}{\partial y} \right)$$
(47)

$$\frac{\partial^2 - \ln \mathcal{P}_{i\mu}^r}{\partial x \, \partial y} = \frac{\partial - \ln \mathcal{P}_{i\mu}^r}{\partial x} \, \frac{\partial - \ln \mathcal{P}_{i\mu}^r}{\partial y} + \tag{48}$$

$$\sum_{k} \mathcal{R}_{i\mu k}^{r} \left( \frac{\partial^{2} - \ln G_{i\mu k}}{\partial x \partial y} - \frac{\partial - \ln G_{i\mu k}}{\partial x} \frac{\partial - \ln G_{i\mu k}}{\partial y} \right)$$
(49)

$$\frac{\partial^2 - \ln \mathcal{P}_i^t}{\partial n_{\mu} \partial n_{\nu}} = \frac{\partial - \ln \mathcal{P}_i^t}{\partial n_{\mu}} \frac{\partial - \ln \mathcal{P}_i^t}{\partial n_{\nu}}$$
(50)

First order derivatives of  $\mathcal{P}_{i\mu}^{v}$ :

$$\frac{\partial -\ln \mathcal{P}_{i\rho}^{\nu}}{\partial n_{\mu}} = -\delta_{\mu\rho} \frac{1}{n_{\mu}} \tag{51}$$

$$\frac{\partial -\ln \mathcal{P}^{v}_{i\rho}}{\partial \vec{r}_{\mu}} = \frac{\partial -\ln \mathcal{P}^{r}_{i\rho}}{\partial \vec{r}_{\mu}} + \frac{\partial -\ln \mathcal{P}^{p}_{i\rho}}{\partial \vec{r}_{\mu}}$$
(52)

$$\frac{\partial - \ln \mathcal{P}_{i\rho}^{r}}{\partial \vec{r}_{\mu}} = \delta_{\mu\rho} \sum_{k} \mathcal{R}_{i\mu k}^{r} \frac{\partial \vec{d}_{i\mu}}{\partial \vec{r}_{\mu}} V_{i}^{-1} \vec{d}_{i\mu}$$
(53)

$$\frac{\partial - \ln \mathcal{P}_{i\rho}^{p}}{\partial \vec{r}_{\mu}} = \left(\delta_{\rho\mu} - \delta_{\rho-1,\mu}\right) \frac{\vec{p}_{\perp}}{|\Delta \vec{r}_{\rho}|} \left(\frac{\partial - \ln \mathcal{P}_{i\rho}^{p}}{\partial p_{z}} - 2 p_{z} \frac{\partial - \ln \mathcal{P}_{i\rho}^{p}}{\partial p_{\perp}^{2}}\right)$$
(54)

(55)

Second order derivatives of  $\mathcal{P}_{iu}^v$ :

$$\frac{\partial^2 - \ln \mathcal{P}^{v}_{i\rho}}{\partial n_{\mu} \partial n_{\nu}} = \delta_{\delta\mu\nu} \frac{1}{n_{\mu}^2} \tag{56}$$

$$\frac{\partial^2 - \ln \mathcal{P}^{v}_{i\rho}}{\partial \vec{r}_{\mu} \, \partial n_{\nu}} = 0 \tag{57}$$

$$\frac{\partial^2 - \ln \mathcal{P}^{v}_{i\rho}}{\partial \vec{r}_{\mu} \, \partial \vec{r}_{\nu}} = \frac{\partial^2 - \ln \mathcal{P}^{r}_{i\rho}}{\partial \vec{r}_{\mu} \, \partial \vec{r}_{\nu}} + \frac{\partial^2 - \ln \mathcal{P}^{p}_{i\rho}}{\partial \vec{r}_{\mu} \, \partial \vec{r}_{\nu}}$$
(58)

$$\frac{\partial^2 - \ln G_{i\rho k}}{\partial \vec{r}_{\mu} \, \partial \vec{r}_{\nu}} = \delta_{\mu\nu\rho} \frac{\partial \vec{d}_{i\mu}}{\partial \vec{r}_{\mu}} V_{ik}^{-1} \frac{\partial \vec{d}_{i\mu}}{\partial \vec{r}_{\nu}}$$
(59)

$$\frac{\partial^2 - \ln \mathcal{P}^{p_{\perp}}_{i\rho}}{\partial \vec{r}_{\cdot}^{i} \partial \vec{r}_{\nu}^{j}} = (\delta_{\rho\mu} - \delta_{\rho-1,\mu}) (\delta_{\rho\nu} - \delta_{\rho-1,\nu})$$

$$(60)$$

$$\left\{ \frac{\partial^2 p_{\perp}^2}{\partial \Delta \vec{r_{\rho}}^i \partial \Delta \vec{r_{\rho}}^j} \frac{\partial - \ln \mathcal{P}_{i\rho}^p}{\partial p_{\perp}^2} + 4 p_z^2 \frac{\vec{p_{\perp}}^i \vec{p_{\perp}}^j}{|\Delta \vec{r_{\rho}}|^2} \frac{\partial^2 - \ln \mathcal{P}_{i\rho}^p}{\partial p_{\perp}^2 \partial p_{\perp}^2} \right\}$$
(61)

$$\frac{\partial^2 - \ln \mathcal{P}_{i\rho}^{p_z}}{\partial \vec{r}^{\,i} \partial \vec{r}_{,i}^{\,j}} = (\delta_{\rho\mu} - \delta_{\rho-1,\mu}) \left( \delta_{\rho\nu} - \delta_{\rho-1,\nu} \right) \tag{62}$$

$$\left\{ \frac{\partial^{2} p_{z}}{\partial \Delta \vec{r_{\rho}}^{i} \partial \Delta \vec{r_{\rho}}^{j}} \frac{\partial - \ln \mathcal{P}_{i\rho}^{p}}{\partial p_{z}} + \frac{\vec{p_{\perp}}^{i} \ \vec{p_{\perp}}^{j}}{|\Delta \vec{r_{\rho}}|^{2}} \frac{\partial^{2} - \ln \mathcal{P}_{i\rho}^{p}}{\partial p_{z} \partial p_{z}} \right\}$$
(63)

Relations for the vertex correlation.

$$\Delta \vec{r}_{\mu} = \vec{r}_{\mu} - \vec{r}_{\mu-1} \tag{64}$$

$$p_z = \frac{\vec{p} \, \Delta \vec{r}}{|\Delta \vec{r}|} \tag{65}$$

$$p_{\perp}^{2} = p^{2} - \left(\frac{\vec{p} \, \Delta \vec{r}}{|\Delta \vec{r}|}\right)^{2} \tag{66}$$

$$\frac{\partial p_z}{\partial \Delta \vec{r}_{\mu}} = \frac{\vec{p}_{\perp}}{|\Delta \vec{r}_{\mu}|} \tag{67}$$

$$\frac{\partial p_{\perp}^{2}}{\partial \Delta \vec{r}_{\mu}} = -2 p_{z} \frac{\partial p_{z}}{\partial \Delta \vec{r}_{\mu}} = -2 p_{z} \frac{\vec{p}_{\perp}}{|\Delta \vec{r}_{\mu}|}$$
(68)

$$\frac{\partial^{2} p_{z}}{\partial \Delta \vec{r}_{\mu}^{i} \partial \Delta \vec{r}_{\mu}^{j}} = \frac{p_{z}}{|\Delta \vec{r}_{\mu}|^{2}} \left( \frac{\Delta \vec{r}_{\mu}^{i} \Delta \vec{r}_{\mu}^{j}}{|\Delta \vec{r}_{\mu}|^{2}} - \delta_{ij} \right) - \frac{\vec{p}_{\perp}^{i} \Delta \vec{r}_{\mu}^{j} + \vec{p}_{\perp}^{j} \Delta \vec{r}_{\mu}^{i}}{|\Delta \vec{r}_{\mu}|^{3}}$$
(69)

$$\frac{\partial^2 p_{\perp}^2}{\partial \Delta \vec{r}_{,i} \partial \Delta \vec{r}_{,i}^{j}} = -2 \frac{\vec{p}_{\perp}^{i}}{|\Delta \vec{r}_{\mu}|} \frac{\vec{p}_{\perp}^{j}}{|\Delta \vec{r}_{\mu}|} - 2 p_z \frac{\partial^2 p_z}{\partial \Delta \vec{r}_{,i}^{i} \partial \Delta \vec{r}_{,i}^{j}}$$
(70)

$$\frac{\partial f_{\mu}}{\partial \vec{r}_{\nu}} = (\delta_{\mu\nu} - \delta_{\mu-1,\nu}) \frac{\partial f_{\mu}}{\partial \Delta \vec{r}_{\mu}}$$
 (71)

$$\frac{\partial f_{\mu}}{\partial \Delta \vec{r}_{\mu}} = \frac{\vec{p}_{\perp}}{|\Delta \vec{r}_{\mu}|} \frac{\partial f}{\partial p_{z}} \tag{72}$$

$$\frac{\partial^2 f_{\mu}}{\partial \Delta \vec{r}_{\mu}^{\ i} \partial \Delta \vec{r}_{\mu}^{\ j}} = \frac{\partial^2 p_z}{\partial \Delta \vec{r}_{\mu}^{\ i} \partial \Delta \vec{r}_{\mu}^{\ j}} \frac{\partial f}{\partial p_z} + \frac{\vec{p}_{\perp}^{\ i} \ \vec{p}_{\perp}^{\ j}}{|\Delta \vec{r}_{\mu}|^2} \frac{\partial^2 f}{\partial p_z \partial p_z}$$
(73)

# A.3 First and second order derivatives of $-\ln \mathcal{L}^c$

$$\mathcal{L} = \mathcal{L}^t \cdot \mathcal{L}^c \tag{75}$$

(74)

$$\mathcal{L} = \mathcal{L} \cdot \mathcal{L}$$

$$\mathcal{L}^{c} = \prod_{\mu} \mathcal{P}^{\nu}_{\mu} \mathcal{P}^{dir}_{\mu} \mathcal{P}^{life}_{\mu}$$

$$(76)$$

$$\mathcal{P}^{v}_{\mu}(\vec{r}_{\mu}) = \frac{1}{(2\pi)^{1.5}\sqrt{|V_{\mu}|}} \exp\left(-\frac{1}{2}(\vec{r}_{\mu} - \vec{r}^{e}_{\mu})V^{-1}_{\mu}(\vec{r}_{\mu} - \vec{r}^{e}_{\mu})\right)$$
(77)

$$\mathcal{P}_{\mu}^{life}(\Delta \vec{r}_{\mu}) = \frac{1}{x_{\mu}} e^{-\Delta \vec{r}_{\mu}/x_{\mu}} \tag{78}$$

$$\mathcal{P}_{\mu}^{dir}(\Delta \vec{r}_{\mu}) = \frac{1}{2\pi\sigma_{\alpha}} \exp\left(-\frac{\alpha_{\mu}^{2}}{2\sigma_{\alpha_{\mu}}}\right)$$
 (79)

$$\cos \alpha_{\mu} = \frac{\Delta \vec{r}_{\mu} \cdot \vec{u}_{\mu}}{|\Delta \vec{r}_{\mu}|} \tag{80}$$

$$\sin \alpha_{\mu} = \frac{\Delta \vec{r}_{\mu} \cdot \vec{u}_{\perp \mu}}{|\Delta \vec{r}_{\mu}|} \tag{81}$$

$$|\vec{u}_{(\perp)\mu}| = 1 \tag{82}$$

Derivatives:

$$\frac{\partial -\ln \mathcal{P}^{v}_{\mu}}{\partial \vec{r}_{\mu}} = V^{-1}_{\mu}(\vec{r}_{\mu} - \vec{r}^{e}_{\mu}) \tag{83}$$

$$\frac{\partial^2 - \ln \mathcal{P}^{\nu}_{\mu}}{\partial \vec{r}^{i}_{\mu} \partial \vec{r}^{j}_{\mu}} = V_{\mu}^{-1} \tag{84}$$

$$\frac{\partial - \ln \mathcal{P}_{\mu}^{life}}{\partial \Delta \vec{r}_{\mu}} = \frac{\Delta \vec{r}_{\mu}}{x_{\mu} |\Delta \vec{r}_{\mu}|} \tag{85}$$

$$\frac{\partial^2 - \ln \mathcal{P}_{\mu}^{life}}{\partial \Delta \vec{r}_{\mu}^{i} \partial \Delta \vec{r}_{\mu}^{j}} = \frac{\delta_{ij}}{x_{\mu} |\Delta \vec{r}_{\mu}|} - \frac{\Delta \vec{r}_{\mu}^{i} \Delta \vec{r}_{\mu}^{j}}{x_{\mu} |\Delta \vec{r}_{\mu}|^{3}}$$
(86)

$$\frac{\partial - \ln \mathcal{P}_{\mu}^{dir}}{\partial \Delta \vec{r}_{\mu}} = \frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}} \frac{\alpha_{\mu}}{2\sigma_{\alpha_{\mu}}}$$
(87)

$$\frac{\partial^{2} - \ln \mathcal{P}_{\mu}^{dir}}{\partial \Delta \vec{r}_{\mu}^{i} \partial \Delta \vec{r}_{\mu}^{j}} = \left( \alpha_{\mu} \frac{\partial^{2} \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{i} \partial \Delta \vec{r}_{\mu}^{j}} + \frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{i}} \frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{j}} \right) \frac{1}{\sigma_{\alpha_{\mu}}^{2}}$$
(88)

$$\frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}} = \frac{1}{\cos \alpha_{\mu}} \frac{\vec{u}_{\perp \mu}}{|\Delta \vec{r}_{\mu}|} - \tan \alpha_{\mu} \frac{\Delta \vec{r}_{\mu}}{|\Delta \vec{r}_{\mu}|^{2}}$$
(89)

$$\frac{\partial^{2} \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{i} \partial \Delta \vec{r}_{\mu}^{j}} = \tan \alpha_{\mu} \left( 3 \frac{\Delta \vec{r}_{\mu}^{i} \Delta \vec{r}_{\mu}^{j}}{|\Delta \vec{r}_{\mu}|^{4}} - \frac{\delta_{ij}}{|\Delta \vec{r}_{\mu}|^{2}} + \frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{i}} \frac{\partial \alpha_{\mu}}{\partial \Delta \vec{r}_{\mu}^{j}} \right)$$
(90)

$$-\frac{1}{\cos\alpha_{\mu}}\frac{\vec{u}_{\perp\mu}^{i}\Delta\vec{r}_{\mu}^{j} + \vec{u}_{\perp\mu}^{j}\Delta\vec{r}_{\mu}^{i}}{|\Delta\vec{r}_{\mu}|^{4}} \tag{91}$$