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TITLE: LINEAR FITTING OF BPM ORBITS AND LATTICE PARAMETERS*

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I. Introduction

The BPM orbits in an accelerator provide two kinds of important information:

- Trajectory parameters if the lattice between the used BPMs is known.
- Lattice parameters if the trajectory parameters are known.

The parameters can be induced from fits to the BPM data. The two scenarios are, however, very different in their statistical nature in the case of small signal-to-noise ratios on the BPM readings. For the fit of trajectory parameters, one needs the knowledge of BPM locations and lattice parameters, i.e. quantities which have no stochastic errors. Standard χ^2 -fits turn out to be appropriate in this case. For the fit of lattice parameters, however, one has to correlate BPM data with trajectory parameters, i.e. quantities which will in general have significant stochastic noise components. This is of great importance for online monitoring purposes, where trajectory parameters themselves have to be induced from BPM readings and have only relatively small variations, solely due to natural orbit and energy fluctuations. In this case, the fit must take into account the noise on the measured trajectory parameters due to finite BPM resolution.

This is illustrated in Fig. 1. If a simple straight line fit $y = px + q$ is applied to data-samples which are linearly correlated but smeared stochastically in both coordinates, the slope is systematically underestimated. The figure shows the ratio of the average reconstructed slope p and the real slope p_0 as a function of the signal-to-noise ratio R_x in the x -coordinate, i.e. the ratio of the real variation of the x -signal as compared to its stochastic noise. Systematic effects are serious up to relatively large R_x . At $R_x = 3$ the inaccuracy is still 10%. Note that this result does not depend on the signal-to-noise ratio in the y -component. A consequence of this bias is that the fit of the x, y -correlation will give different results depending on whether y is fitted as a function of x , or x as a function of y . An explicit example is given in Fig. 2 where 100 data-points were generated with a signal-to-noise ratio $R_x = 1$ and a slope $p_0 = 1$. The χ^2 -fit reconstructs $p = 0.50 \pm 0.03$ which deviates from p_0 by a factor 2. The result from the alternative fitting technique, described in this note, is also shown in Fig. 2 (see chapter IV).

This behavior is relevant for many online correlation-plot applications in which BPM readings, or other quantities with stochastic noise, are being correlated. Linear least χ^2 -fits will in general give wrong results since the errors are not properly handled.

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In this note we discuss a solution for this problem. Chapter II covers briefly the standard χ^2 -fitting of trajectory parameters. Chapter III discusses the case of linear correlations between independent measurements which are all subject to stochastic noise. An analytic solution for unbiased fits including the error analysis is derived. Examples are presented in chapter IV.

The mathematical analysis in chapter III is involved and possibly not of general interest. The algorithms for fitting and error analysis can, however, be extracted by using equations (17), (32), (33) alone.

The fit methods are available as general software packages (written in MATLAB code) on the MCC/SLC-VAX. Similar packages were produced for the HP 28 S pocket calculator for testing purposes. The methods were successfully applied for online monitoring of dispersion functions and transfer-matrix elements.

II. Trajectory Parameters from Known Lattices

In this case, the position measurement $x(s)$ of a BPM at longitudinal position s can be written as a superposition of sine-like and cosine-like betatron oscillations and the dispersion function:

$$x(s) = A \sqrt{\beta(s)} \sin \Phi(s) + B \sqrt{\beta(s)} \cos \Phi(s) + C \eta(s) \quad (1)$$

The parameters A, B, C determine the trajectory. The measurement $x(s)$ has an error due to finite BPM resolutions while the lattice functions $\beta(s), \Phi(s), \eta(s)$ do not.

This scenario can be generalized in the following way: Let $x(s)$ be a linear combination of n known functions $g_1(s), \dots, g_n(s)$

$$x(s) = \sum_{i=1}^n p_i g_i(s) \quad (2)$$

where $\mathbf{p} = (p_1, \dots, p_n)^T$ is a vector of n parameters of interest. Let $x_\nu \pm \sigma_\nu$ be measurements at N "positions" s_ν . Then the problem of determining $\mathbf{p}$ reduces to a simple χ^2 -fit:

$$\chi^2 = \sum_{\nu=1}^N \frac{1}{\sigma_\nu^2} \left(x_\nu - \sum_{i=1}^n p_i g_i(s_\nu) \right)^2 = \text{Min} . \quad (3)$$

The solution to this can be obtained by solving $\nabla_{\mathbf{p}} \chi^2(\mathbf{p}) = 0$ and is well known: Define normalized coordinates $\mathbf{z} = (z_1, \dots, z_N)^T$ by

$$z_\nu = \frac{x_\nu}{\sigma_\nu} \quad (4)$$

and the $N \times n$ matrix $\mathbf{B}$ by

$$B_{\nu i} = \frac{g_i(s_\nu)}{\sigma_\nu} . \quad (5)$$

After defining the covariance matrix

$$\mathbf{T} = (\mathbf{B}^T \cdot \mathbf{B})^{-1}, \quad (6)$$

the solution reads

$$\mathbf{p} = \mathbf{T} \cdot \mathbf{B}^T \cdot \mathbf{z} \quad (7)$$

$$\chi^2 = \mathbf{z}^T \cdot \mathbf{z} - \mathbf{z}^T \cdot \mathbf{B} \cdot \mathbf{T} \cdot \mathbf{B}^T \cdot \mathbf{z}.$$

The error of any scalar function $f(\mathbf{p})$ of the parameters $\mathbf{p}$ is given by

$$\sigma(f)^2 = (\nabla_{\mathbf{p}} f)^T \cdot \mathbf{T} \cdot (\nabla_{\mathbf{p}} f). \quad (8)$$

The errors of the parameters themselves are determined by the diagonal elements of $\mathbf{T}$ alone,

$$\sigma(p_i) = \sqrt{T_{ii}}, \quad (9)$$

which follows from (8) in the special case $f(\mathbf{p}) = p_i$.

III. Lattice Parameters for Known Trajectories

The position measurement $x(s)$ of a BPM at longitudinal position s may be correlated with the trajectory parameters $x, x', \frac{\delta E}{E}$ at another position s_0 using the transfer matrix $\mathbf{R}$ (we use TRANSPORT notation):

$$x(s) = R_{11}^{(s_0:s)} x(s_0) + R_{12}^{(s_0:s)} x'(s_0) + R_{16}^{(s_0:s)} \frac{\delta E}{E} \quad (10a)$$

In this case the lattice parameters $R_{11}^{(s_0:s)}, R_{12}^{(s_0:s)}, R_{16}^{(s_0:s)}$ can be fitted with the method in chapter II if the trajectory parameters $x(s_0), x'(s_0), \frac{\delta E}{E}$ are known with infinite precision. In general, however, this condition will not be fulfilled. If, for example, $x(s_0), x'(s_0), \frac{\delta E}{E}$ are inferred from the information $x^{(1)}, x^{(2)}, x^{(3)}$ of 3 appropriate BPMs, the trajectory parameters carry the same uncertainty (BPM resolution errors) as the measurement $x(s)$ itself. This becomes more obvious if equation (10a) is rewritten directly in terms of the independent BPM readings:

$$Ax + Bx^{(1)} + Cx^{(2)} + Dx^{(3)} = 0 \quad (10b)$$

The quantities $x(s_0), x'(s_0)$ and $\frac{\delta E}{E}$ are linear combinations of $x^{(1)}, x^{(2)}, x^{(3)}$. The parameters $R_{11}^{(s_0:s)}, R_{12}^{(s_0:s)}$ and $R_{16}^{(s_0:s)}$ are, correspondingly, linear combinations of $-\frac{B}{A}, -\frac{C}{A}, -\frac{D}{A}$. Geometrically, equation (10b) describes a 3-dimensional hyperplane in 4-dimensional space $(x, x^{(1)}, x^{(2)}, x^{(3)})$. The parameter-vector $(A, B, C, D)^T$ points perpendicular to this hyperplane. The minimization problem is to orient this parameter-vector such that the distances of the measured data points (in units of standard deviations) to the hyperplane are minimized in a least square sense. Pictorially, we therefore have to find the "principal axes of the set of data-points", and then turn the parameter-vector parallel to the principal axis along which the data-points fluctuate the least.

We shall discuss a generalization of this scenario here. Let x_n be a measurement which is linearly correlated to $n - 1$ other measurements $x_1, \dots, x_{n-1}$. Let all the measurements carry uncorrelated random resolution errors, called $\sigma_1, \dots, \sigma_n$. The fit problem is hence to find a hyperplane in $\mathbb{R}^n$ with smallest distance to a given set of N measurements (which are points in $\mathbb{R}^n$). Defining normalized coordinates

$$z_i = \frac{x_i - \langle x_i \rangle}{\sigma_i}, \quad (11)$$

the shortest distance (measured in standard deviations) of a single measurement $\mathbf{z}_\nu = (z_{\nu 1}, \dots, z_{\nu n})^T$ to this hyperplane is given by

$$d_u(\mathbf{z}_\nu) = |\mathbf{u}^T \cdot \mathbf{z}_\nu| \quad (12)$$

where $\mathbf{u}$ is a unity-vector perpendicular to the hyperplane. Minimizing

$$\chi^2(\mathbf{u}) = \sum_{\nu=1}^N (\mathbf{u}^T \cdot \mathbf{z}_\nu)^2 \quad (13)$$

hence solves the fit equation

$$\mathbf{u}^T \cdot \mathbf{z} = 0 \quad (14)$$

in a least square sense and solves the problem (using (11)).

The χ^2 function in (13) has an overall scale which is fixed by the fact that $\mathbf{u}$ is a unity-vector. By introducing a Lagrange multiplier λ , we can insert this constraint and arrive at the minimization problem

$$\chi^2(\mathbf{u}, \lambda) = \sum_{\nu=1}^N (\mathbf{u}^T \cdot \mathbf{z}_\nu)^2 + \lambda(1 - \mathbf{u}^T \cdot \mathbf{u}) = \text{Min} . \quad (15)$$

After defining the positive definite symmetric $n \times n$ (covariance) matrix $\mathbf{C}$ by

$$C_{ij} = \sum_{\nu=1}^N z_{\nu i} z_{\nu j} , \quad (16)$$

equation (15) leads to

$$\begin{aligned} \mathbf{C} \cdot \mathbf{u} &= \lambda \mathbf{u} \\ |\mathbf{u}|^2 &= 1 \\ \chi^2 &= \lambda . \end{aligned} \quad (17)$$

Therefore the solution of the fit is simply the normalized eigenvector $\mathbf{u}$ corresponding to the smallest eigenvalue λ of the covariance matrix $\mathbf{C}$. The eigenvalue λ is also the χ^2 of the fit.

However, the error analysis for u is not straightforward: Let $\lambda_1, \dots, \lambda_n$ be the n eigenvalues of C and let $u_1, \dots, u_n$ be the corresponding eigenvectors. We assume that $\lambda = \lambda_1$ is the smallest eigenvalue and that it is not degenerate (otherwise u is not uniquely defined and errors diverge unless the redundant parameters in the fit are eliminated). The solution is then $u = u_1$. It is well known that the eigenvectors can always be chosen to be orthonormal and the $n \times n$ matrix O defined by

$$O_{ij} = (u_j)_i \quad (18)$$

is orthogonal and diagonalizes C :

$$O^T \cdot C \cdot O = O \cdot O^T = I \quad (19a)$$

$$O^T \cdot C \cdot O = D = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_n \end{pmatrix} \quad (19b)$$

A consequence of (18) and (19a) is

$$\begin{aligned} O^T \cdot u_j &= e_j \\ O \cdot e_j &= u_j \end{aligned} \quad (20)$$

(The vector e_j is the unity-vector in j -direction and I is the $n \times n$ unity-matrix).

If the matrix C changes by dC due to a variation in the measurements, both the eigenvalue $\lambda = \lambda_1$ and the eigenvector $u = u_1$ change (by $d\lambda$ and du , respectively):

$$dC \cdot u + C \cdot du = d\lambda u + \lambda du \quad (21)$$

Since u must remain normalized, u and its variation du are orthogonal:

$$u^T \cdot du = \frac{1}{2} d(|u|^2) = 0 \quad (22)$$

Multiplying (21) by u^T and using (22) we get

$$u^T \cdot dC \cdot u + u^T \cdot C \cdot du = d\lambda ,$$

but because of $u^T \cdot C = \lambda u^T$ and (22)

$$u^T \cdot C \cdot du = 0 .$$

We therefore arrive at

$$d\lambda = \mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u} . \quad (23)$$

Plugging this into (21) we find

$$(\mathbf{C} - \lambda \mathbf{I}) \cdot d\mathbf{u} = [(\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{I} - d\mathbf{C}] \cdot \mathbf{u} ,$$

and using (19a)

$$\mathbf{O}^T \cdot (\mathbf{C} - \lambda \mathbf{I}) \cdot \mathbf{O} \cdot \mathbf{O}^T \cdot d\mathbf{u} = \mathbf{O}^T \cdot [(\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{I} - d\mathbf{C}] \cdot \mathbf{u} .$$

Using (19b) and (20) this means

$$\begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & \lambda_2 - \lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n - \lambda \end{pmatrix} \cdot \mathbf{O}^T \cdot d\mathbf{u} = (\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{e}_1 - \mathbf{O}^T \cdot d\mathbf{C} \cdot \mathbf{u} . \quad (24)$$

The first row in this system of equations is an empty equation ($0 = 0$). To solve (24) uniquely we must use (22) in addition:

$$0 = \mathbf{u}^T \cdot d\mathbf{u} = \mathbf{u}^T \cdot \mathbf{O} \cdot \mathbf{O}^T \cdot d\mathbf{u} = \mathbf{e}_1^T \cdot \mathbf{O}^T \cdot d\mathbf{u}$$

Adding this into the first row of (24) we get

$$\begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \lambda_2 - \lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n - \lambda \end{pmatrix} \cdot \mathbf{O}^T \cdot d\mathbf{u} = (\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{e}_1 - \mathbf{O}^T \cdot d\mathbf{C} \cdot \mathbf{u} . \quad (25)$$

Defining the diagonal $n \times n$ matrix

$$\Lambda = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \frac{1}{\lambda_2 - \lambda} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{\lambda_n - \lambda} \end{pmatrix} \quad (26)$$

(which exists since $\lambda = \lambda_1$ is not degenerate) we can write the solution of (25) as

$$\mathbf{O}^T \cdot d\mathbf{u} = (\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{e}_1 - \Lambda \cdot \mathbf{O}^T \cdot d\mathbf{C} \cdot \mathbf{u} ,$$

where we used $\Lambda \cdot \mathbf{e}_1 = \mathbf{e}_1$. This means

$$d\mathbf{u} = (\mathbf{u}^T \cdot d\mathbf{C} \cdot \mathbf{u})\mathbf{u} - \mathbf{O} \cdot \Lambda \cdot \mathbf{O}^T \cdot d\mathbf{C} \cdot \mathbf{u} \quad (27)$$

which connects the errors in the parameters $\mathbf{u}$ explicitly with the errors in the matrix $\mathbf{C}$.

Since $\mathbf{C}$ is symmetric, it has $\frac{1}{2}n(n+1)$ independent components (C_{ij} with $i \leq j$). Varying C_{ij} hence affects 2 elements in $\mathbf{C}$ if $i \neq j$:

$$\frac{\partial \mathbf{C}}{\partial C_{ij}} = \frac{1}{1 + \delta_{ij}} (\mathbf{e}_i \cdot \mathbf{e}_j^T + \mathbf{e}_j \cdot \mathbf{e}_i^T) . \quad (28)$$

From (27) we hence derive:

$$(1 + \delta_{ij}) \frac{\partial u_l}{\partial C_{ij}} = 2u_i u_j u_l - \sum_{r=1}^n O_{lr} \Lambda_{rr} (O_{ir} u_j + O_{jr} u_i) \quad (29)$$

Let $f(\mathbf{u})$ be any scalar function of the fit parameters. The error of f reads:

$$\sigma(f)^2 = \sum_{\nu=1}^N \sum_{j=1}^n \left(\frac{\partial f}{\partial z_{\nu j}} \right)^2 = \sum_{i,j=1}^n \left[\frac{\partial f}{\partial u_i} \frac{\partial f}{\partial u_j} \sum_{k=1}^n \sum_{\nu=1}^N \frac{\partial u_i}{\partial z_{\nu k}} \frac{\partial u_j}{\partial z_{\nu k}} \right] \quad (30)$$

where we used the fact that $\sigma(z_{\nu j})^2 = 1$ (normalized coordinates). Using (16) we derive

$$\begin{aligned} \frac{\partial u_l}{\partial z_{\nu k}} &= \sum_{i=1}^n \sum_{j=1}^n \frac{\partial u_l}{\partial C_{ij}} \frac{\partial C_{ij}}{\partial z_{\nu k}} = \sum_{i=1}^n \sum_{j=1}^n \frac{\partial u_l}{\partial C_{ij}} (z_{\nu i} \delta_{jk} + z_{\nu j} \delta_{ik}) \\ &= \sum_{i=1}^k \frac{\partial u_l}{\partial C_{ik}} z_{\nu i} + \sum_{j=k}^n \frac{\partial u_l}{\partial C_{kj}} z_{\nu j} = \sum_{i=1}^n \frac{\partial u_l}{\partial C_{ik}} z_{\nu i} (1 + \delta_{ik}) \end{aligned}$$

which together with (29) becomes

$$\frac{\partial u_l}{\partial z_{\nu k}} = \sum_{i=1}^n z_{\nu i} \left[2u_i u_k u_l - \sum_{r=1}^n O_{ir} \Lambda_{rr} (O_{ir} u_k + O_{kr} u_i) \right] . \quad (31)$$

Hence with (17)-(20):

$$\begin{aligned} \sum_{k=1}^n \sum_{\nu=1}^N \frac{\partial u_i}{\partial z_{\nu k}} \frac{\partial u_j}{\partial z_{\nu k}} &= \sum_{k=1}^n \sum_{l,m=1}^n C_{lm} \left[2u_i u_k u_l - \sum_{r=1}^n O_{ir} \Lambda_{rr} (O_{ir} u_k + O_{kr} u_l) \right] \times \\ &\quad \times \left[2u_m u_k u_j - \sum_{s=1}^n O_{js} \Lambda_{ss} (O_{ms} u_k + O_{ks} u_m) \right] \\ &= 4\lambda u_i u_j - 2\lambda(2u_i u_j) - 2\lambda(2u_i u_j) + \sum_{r=1}^n \left[O_{ir} O_{jr} (\lambda_r \Lambda_{rr}^2 + 2\lambda \delta_{r1} + \lambda \Lambda_{rr}^2) \right] \\ &= \sum_{r=2}^n O_{ir} O_{jr} \Lambda_{rr}^2 (\lambda_r + \lambda) \\ &= \sum_{r=2}^n \frac{\lambda_r + \lambda}{(\lambda_r - \lambda)^2} (\mathbf{u}_r)_i (\mathbf{u}_r)_j \end{aligned}$$

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Introducing this into (30) we get the answer

$$\sigma(f)^2 = (\nabla_u f)^T \cdot T \cdot (\nabla_u f) . \quad (32)$$

where T is a symmetric $n \times n$ matrix defined by

$$T_{ij} = \sum_{r=2}^n \frac{\lambda_r + \lambda}{(\lambda_r - \lambda)^2} (u_r)_i (u_r)_j . \quad (33)$$

The equations (32), (33) allow the complete error analysis knowing the eigenvalues $\lambda_1, \dots, \lambda_n$ and eigenvectors $u_1, \dots, u_n$.

IV. Examples

A simple example of the fitting procedures is given in Fig. 2. Data points were generated in the (x, y) plane around a straight line of slope 1 and then smeared randomly, both in x and y , by fixed resolution errors σ_x, σ_y . The signal-to-noise ratio R_x was chosen to be $R_x = 1$. The principal axis transformation, described in chapter III, reconstructs the straight line correctly within errors. Using a direct χ^2 -fit of the relation $y = px + q$, however, leads to an underestimation of the slope p by about a factor of 2, and in addition, the error on p is drastically underestimated. This is exactly the expectation from Fig. 1 and a direct consequence of neglecting the horizontal smearing of the data due to the finite resolution σ_x .

An example of practical interest is shown in Fig. 3 where lattice parameters R_{10} , R_{11} and R_{12} are reconstructed for the Final Focus System using equations (10a,b). We simulated 100 trajectories with fluctuations in the energy and the betatron-orbit. The lattice parameters are inferred from these variations alone. All BPM measurements were smeared stochastically according to a finite resolution of $20\mu m$. As can be seen from Fig. 3 the lattice parameters are reconstructable using the principal axes transformation. A direct χ^2 -fit of the lattice parameters, however, leads to seemingly good fits with small errors which nevertheless are in violent disagreement with the model-parameters used for the trajectory generation.

Figure Captions

- Fig. 1 :** Systematic slope error introduced in a simple linear χ^2 -fit of the form $y = px + q$ in which the noise smearing in the measurements for x is neglected. Shown is the reconstructed slope p normalized to the true slope p_0 as function of the signal-to-noise ratio, R_x , in the horizontal coordinate.
- Fig. 2 :** Data points in the (x, y) -plane generated along the straight line $y = x + 10$ and smeared according to uncorrelated noise errors $\sigma_x = 1, \sigma_y = 0.5$. The signal-to-noise ratios were chosen to be 1 for x and 2 for y . The results of the fits described in chapters II and III are indicated.
- Fig. 3 :** Reconstructed Final Focus lattice parameters R_{10}, R_{11}, R_{12} from a sample of 100 simulated trajectories with fluctuations in energy and betatron-orbits assuming a BPM noise of $20\mu m$. The methods described in chapters II (Fig. 3a) and III (Fig. 3b) are compared to the model parameters used for the trajectory generation.

RMS-R=20.000 um
RMS-E=5.000 /mil
RMS-U=5.000, RMS-V=5.000

Fig 3a

sigma Beta = 3023.82 um
sigma dE/E = 5.09 /mil

RMS-R=20.000 um
RMS-E=5.000 /mil
RMS-U=5.000, RMS-V=5.000

Fig 3b

sigma Beta = 3023.82 um
sigma dE/E = 5.09 /mil