A HYBRID TECHNIQUE FOR COMPUTING COURANT-SNYDER PARAMETERS FROM BEAM PROFILE DATA*

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Abstract

We develop novel techniques for computing Courant-Snyder (C-S) parameters of a charged-particle beam from profile measurement data. These methods have robust convergence properties by combining both deterministic and non-deterministic methods. The basic ideas is as follows: given a model of the beamline, in the zero space charge case it is possible to compute the C-S parameters directly from profile data using a deterministic, linear-algebraic approach. For finite space charge we either a) iterate this deterministic solution or b) construct a smooth curve of these deterministic solutions starting from the zero-current solution and terminating at the finite-current case. This selects the finite-current solution connected to the zero-current C-S parameters. Both approaches avoid convergence issues associated with fully iterative, non-deterministic methods. The details of the techniques are outlined and an example is presented using data taken from the SNS accelerator.

INTRODUCTION

The objective here is to develop a robust, accurate algorithm for computing C-S parameters from profile measurements with the aim of matching. To date C-S estimation has not successfully matched the SNS MEBT to the DTL using profile data. The current procedure used at SNS consists of a numerical solver driving a simulation engine; the solver searches for the C-S parameters that minimize error between simulation and measurements. We call this *data fitting*. The advantage is that it is easy to implement, the disadvantage is its weakly defined solution and convergence properties, especially with space charge.

Our new techniques are motivated by direct methods for computing C-S parameters in the zero-current case, see for example [1]. The least-square solution is computed directly from measurements, without minimization. With space charge this direct method serves as the engine for a *fixed-point* iteration scheme. A function is defined whose fixed point is the finite-current solution. The fixed-point method then drives a *continuation method* that constructs a curve of solutions from zero-current to finite-current.

Background

We briefly outline the problem domain primarily to establish the notation. For brevity we focus on horizontal phase space with coordinates $\mathbf{x} \triangleq (x, x') \in \mathbb{R}^2$. Results generalize to the 6D case. Let $\langle\cdot\rangle : L_\infty(\mathbb{R}^2) \to \mathbb{R}$ be the *moment operator* with respect to the beam distribution. For ellipsoidally symmetric beams the second-order moments $\{\langle x^2\rangle, \langle xx'\rangle, \langle x'^2\rangle\}$ and the C-S parameters $\{\alpha, \beta, \epsilon\}$ are equivalent representations [2]. The moments are elements of the symmetric *covariance matrix* $\boldsymbol{\sigma}$

$$\boldsymbol{\sigma} \triangleq \langle \mathbf{x}\cdot\mathbf{x}^T\rangle = \begin{pmatrix} \langle x^2\rangle & \langle xx'\rangle \\ \langle xx'\rangle & \langle x'^2\rangle \end{pmatrix}, \qquad (1)$$

where $\det\boldsymbol{\sigma} = \epsilon^2$, $\langle x^2\rangle = \beta\epsilon$, and $\langle xx'\rangle = -\alpha\epsilon$. We consider only discrete locations $\{s_n\}$ along the beamline and the coordinates $\{\mathbf{x}_n\}$ at those locations. Propagation is modeled via *transfer matrices* $\{\boldsymbol{\Phi}_n\}$ where $\mathbf{x}_{n+1} = \boldsymbol{\Phi}_n\mathbf{x}_n$. Matrix multiplication and the moment operator commute, thus the covariance matrix propagates according to $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\Phi}_n\boldsymbol{\sigma}_n\boldsymbol{\Phi}_n^T$, verified by propagating Eq. (1).

For conciseness we make several definitions. First is the operator T_n given by the action

$$\boldsymbol{\sigma}_{n+1} = T_n(\boldsymbol{\sigma}_0) \triangleq (\boldsymbol{\Phi}_n \cdots \boldsymbol{\Phi}_0)\boldsymbol{\sigma}_0(\boldsymbol{\Phi}_n \cdots \boldsymbol{\Phi}_0)^T, \qquad (2)$$

that is, T_n propagates $\boldsymbol{\sigma}_0$ to $\boldsymbol{\sigma}_{n+1}$. Now let $\mathrm{Sym}(\mathbb{R}^{2\times2})$ be the subspace of symmetric matrices in $\mathbb{R}^{2\times2}$. The following elements form a basis for $\mathrm{Sym}(\mathbb{R}^{2\times2})$:

$$\mathbf{e}_1 \triangleq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{e}_2 \triangleq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{e}_3 \triangleq \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad (3)$$

from which Eq. (1) can be expressed $\boldsymbol{\sigma} = \langle x^2\rangle\mathbf{e}_1 + \langle xx'\rangle\mathbf{e}_2 + \langle x'^2\rangle\mathbf{e}_3$. Next, define the coordinate projection operator π_i on $\mathrm{Sym}(\mathbb{R}^{2\times2})$, which selects the i^{th} coordinate of the basis $\{\mathbf{e}_i\}$, specifically,

$$\pi_i(\sigma_1\mathbf{e}_1 + \sigma_2\mathbf{e}_2 + \sigma_3\mathbf{e}_3) \triangleq \sigma_i\,. \qquad (4)$$

For example, $\pi_1(\boldsymbol{\sigma}) = \langle x^2\rangle$. Finally, it can be shown from the mapping $\boldsymbol{\sigma} \mapsto (\langle x^2\rangle, \langle xx'\rangle, \langle x'^2\rangle)$ that $\mathrm{Sym}(\mathbb{R}^{2\times2}) \cong \mathbb{R}^3$ so $\boldsymbol{\sigma}$ has equivalent representations in either space. When it is necessary to enforce $\boldsymbol{\sigma} \in \mathbb{R}^3$, we denote it by $\vec{\boldsymbol{\sigma}}$. For more information on this material, see [2] and [3].

COURANT-SNYDER ESTIMATION

The *observables* for the C-S estimation problem are the beam sizes $\{\langle x_n^2\rangle\}$ at the N positions $\{s_n\}_{n=1}^N$ along the beamline. The beam sizes are obtained from measurements, for example, wire scanner data. Using the observables the objective is to estimate the *beam state* $\boldsymbol{\sigma}$ at an arbitrary location along the beamline. Pick such a location s_0 and denote the unknown beam state as $\boldsymbol{\sigma}_0$. The $\{T_n\}$ operators provide the model relations $\langle x_{n+1}^2\rangle = \pi_1 \circ T_n(\boldsymbol{\sigma}_0)$, $n = 0, \ldots, N-1$ that link the known beam sizes

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to the unknown beam state $\boldsymbol{\sigma}_0$ at s_0. Expressing $\boldsymbol{\sigma}_0$ as $\langle x_0^2\rangle\mathbf{e}_1 + \langle x_0x_0'\rangle\mathbf{e}_2 + \langle x_0'^2\rangle\mathbf{e}_3$ facilitates the following:

$$\begin{bmatrix}\langle x_1^2\rangle\\ \vdots\\ \langle x_N^2\rangle\end{bmatrix} = \begin{pmatrix}\pi_1\circ T_0(\mathbf{e}_1) & \cdots & \pi_1\circ T_0(\mathbf{e}_3)\\ \vdots & \ddots & \vdots\\ \pi_1\circ T_{N-1}(\mathbf{e}_1) & \cdots & \pi_1\circ T_{N-1}(\mathbf{e}_3)\end{pmatrix}\begin{bmatrix}\langle x_0^2\rangle\\ \langle x_0x_0'\rangle\\ \langle x_0'^2\rangle\end{bmatrix},$$

which we write more compactly in matrix-vector notation

$$\mathbf{m} = \boldsymbol{\Omega}\vec{\boldsymbol{\sigma}}_0\,, \tag{5}$$

where $\mathbf{m} \triangleq [\langle x_1^2\rangle, \ldots, \langle x_N^2\rangle]^T$ is the N-vector of measured beam sizes and $\boldsymbol{\Omega}$ is the $N\times3$ *observation matrix* with elements $[\boldsymbol{\Omega}]_{ij} \triangleq \pi_1\circ T_{i-1}(\mathbf{e}_j)$. Only for the case $N = 3$ is there a potentially unique solution for the above. More typical is the situation $N > 3$ which we consider exclusively. Since the image of $\boldsymbol{\Omega}$ does not cover all of $\mathbb{R}^N$, there are no true solutions in this case. However, we can define the *least-squares solution* $\vec{\boldsymbol{\sigma}}_0^*$ as

$$\vec{\boldsymbol{\sigma}}_0^* \triangleq (\boldsymbol{\Omega}^T\boldsymbol{\Omega})^{-1}\boldsymbol{\Omega}^T\mathbf{m}\,, \tag{6}$$

so named because it minimizes completely the residual error $\|\mathbf{m} - \boldsymbol{\Omega}\vec{\boldsymbol{\sigma}}_0\|_2$ where $\|\cdot\|_2$ is the Lebesgue 2-norm. Specifically, $\vec{\boldsymbol{\sigma}}_0^* = \arg\min_{\vec{\boldsymbol{\sigma}}}\|\mathbf{m} - \boldsymbol{\Omega}\vec{\boldsymbol{\sigma}}\|_2$. If $\boldsymbol{\Omega}$ has full rank then $\vec{\boldsymbol{\sigma}}_0^*$ is well defined. The rank depends upon the model and the measurement setup. Thus, for a well-designed experiment with accurate transfer matrix model Eq. (6) is a reasonable estimate of the C-S parameters at s_0 whenever space charge forces are insignificant.

Estimation with Space Charge

When space charge is significant the transfer matrices $\{\boldsymbol{\Phi}_n\}$ depend upon the second-order moments $\{\boldsymbol{\sigma}_n\}$. Since the transfer matrices are the used to compute $\boldsymbol{\Omega}$, solution relation (6) is transcendental. In general the transfer matrices must now be computed numerically, the details of which are beyond our scope, see [2]. Suffice it to say that they can be formulated to depend upon one moment matrix only, which we *choose* to be $\boldsymbol{\sigma}_0$. Denoting beam charge as q, the dependencies are then represented $\boldsymbol{\Phi}_n = \boldsymbol{\Phi}_n(\boldsymbol{\sigma}_0, q)$, which then implies $\boldsymbol{\Omega} = \boldsymbol{\Omega}(\boldsymbol{\sigma}_0, q)$.

With $\mathbf{m}$ fixed Eq. (6) motivates the definition

$$\mathbf{F}(\vec{\boldsymbol{\sigma}}, q) \triangleq [\boldsymbol{\Omega}^T(\vec{\boldsymbol{\sigma}}, q)\boldsymbol{\Omega}(\vec{\boldsymbol{\sigma}}, q)]^{-1}\boldsymbol{\Omega}^T(\vec{\boldsymbol{\sigma}}, q)\mathbf{m}. \tag{7}$$

We refer to $\mathbf{F}$ as the *reconstruction operator*. It plays the majority role in the remaining analysis. Inspecting Eqs. (6) and (7) note that any fixed point $\vec{\boldsymbol{\sigma}}^*$ of $\mathbf{F}(\cdot, q)$ is a least-squares solution to the C-S estimation problem for beam charge q. One way to exploit this fact is iteration of $\mathbf{F}(\vec{\boldsymbol{\sigma}}, q)$ to its fixed point $\vec{\boldsymbol{\sigma}}^*$.

For ease of notation we discontinue the Gibb's notation for $\boldsymbol{\sigma}$. The first C-S algorithm is a fixed-point method based upon the above iteration scheme. Starting with the known beam charge q^*, a numeric tuning parameter $\alpha \in (0,1)$, and an initial guess $\boldsymbol{\sigma}^0$ for the beam moments, the algorithm iterates according to

$$\boldsymbol{\sigma}^{i+1} = \mathbf{R}(\boldsymbol{\sigma}^i) \triangleq (1-\alpha)\boldsymbol{\sigma}^i + \alpha\mathbf{F}(\boldsymbol{\sigma}^i, q^*) \tag{8}$$

where $\{\boldsymbol{\sigma}^i\}, i = 1,2, \ldots$ are the solution iterates and $\mathbf{R}$ is the *recursion operator*. The parameter α stabilizes the search by governing the distance that $\boldsymbol{\sigma}^{i+1}$ can move from previous value $\boldsymbol{\sigma}^i$. The operator $\mathbf{R}$ also has a fixed point at $\boldsymbol{\sigma}^*$ which can be verified by direct substitution. Suitable choices for $\boldsymbol{\sigma}^0$ and α are $\boldsymbol{\sigma}_0^*$ and ½. It can be shown that if $\|(1-\alpha)\mathbf{I} + \alpha\mathbf{F}'(\boldsymbol{\sigma}^*)\| < 1$ then $\mathbf{R}$ is a contraction at $\boldsymbol{\sigma}^*$ with unique, convergent solution [3].

The second C-S estimation algorithm is based upon continuation; we construct a continuous solution curve $\mathbf{s}(\cdot)$ on the interval $I \triangleq [0, q^*]$ where $\boldsymbol{\sigma}^0 = \mathbf{s}(0) = \boldsymbol{\sigma}_0^*$ is the zero-current solution and $\boldsymbol{\sigma}^* = \mathbf{s}(q^*)$ is the full-current solution (i.e., for the data $\mathbf{m}$). The condition

$$\mathbf{F}[\mathbf{s}(q), q] - \mathbf{s}(q) = 0 \quad \text{for all } q \in \mathrm{I}, \tag{9}$$

the continuity of $\mathbf{F}$, and the fact that $\mathbf{s}(0) = \boldsymbol{\sigma}^0$ is known through Eq. (6), allow the construction of $\mathbf{s}(\cdot)$. Taking the total derivative of Eq. (9) w.r.t. charge q yields

$$\frac{d\mathbf{s}(q)}{dq} = \left[\frac{\partial\mathbf{F}[\mathbf{s}, q]}{\partial\boldsymbol{\sigma}} - \mathbf{I}\right]^{-1}\left[\frac{\partial\mathbf{F}[\mathbf{s}, q]}{\partial q}\right], \tag{10}$$

which is used in the Taylor expansion $\mathbf{s}(q + \Delta q) = \mathbf{s}(q) + d\boldsymbol{s}(q)/dq\,\Delta q + O(\Delta q^2)$. These facts motivate the following solution technique: Divide I into K sub-intervals at locations $\{q^0, q^1, \ldots, q^{K-1} = q^*\}$ then compute $\boldsymbol{\sigma}^{k+1}$ according to the recursion relation

$$\boldsymbol{\sigma}^{k+1} = \boldsymbol{\sigma}^k + \frac{d\mathbf{s}(q^k)}{dq}(q^{k+1} - q^k)\,, \tag{11}$$

where $\boldsymbol{\sigma}^0$ is the zero-current solution of Eq. (6). Note that the number of iterations K is known *a priori*. However, there is more computation per iteration than the previous technique, we must compute the partial derivatives.

It is useful to apply the previous iteration scheme (8) between each of the above recursions to "center" $\boldsymbol{\sigma}^{k+1}$ back onto the solution curve $\mathbf{s}(q^{k+1})$. When $\boldsymbol{\sigma}^k = \mathbf{s}(q^k)$ is augmented by the vector $\Delta\boldsymbol{\sigma}^{k+1}$ the curvature of $\mathbf{s}$ causes $\boldsymbol{\sigma}^k + \Delta\boldsymbol{\sigma}^{k+1}$ to lie outside $\mathbf{s}(\cdot)$. Iteration by Eq. (8) then puts $\boldsymbol{\sigma}^{k+1}$ back on the solution curve at $\mathbf{s}(q^{k+1})$.

Examples

We consider the case of the SNS Medium Energy Beam Transport (MEBT) section that transports a 2.5 MeV H$^-$ beam from an RFQ to the SNS warm linac. Because of low beam energy, space charge forces are prevalent making this an ideal test case. The MEBT consists of a cascade of 14 quadrupole lenses and 4 RF rebunchers. There is an initial bank of 4 wire scanners and 1 additional scanner near the exit. There is also an emittance scanner (EMS) located at 2.45 m from the MEBT entrance. Beam current was 32.5 mA and the pulse train was 45 mini-pulses long (~45 msec).

With the above techniques the C-S parameters were reconstructed at the emittance scanner location. **Figure 1**, **Figure 2**, and **Figure 3** show the solutions computed by each technique; measurements are represented as dots. There was no bunch length data so any longitudinal phase plane solutions were simulated from design specifications.

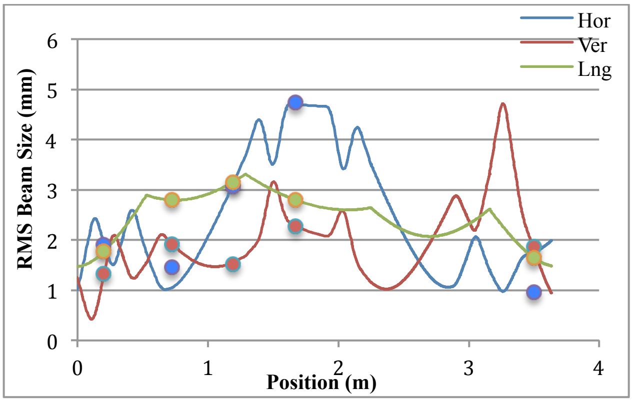

Figure 1: Fixed-point solution.

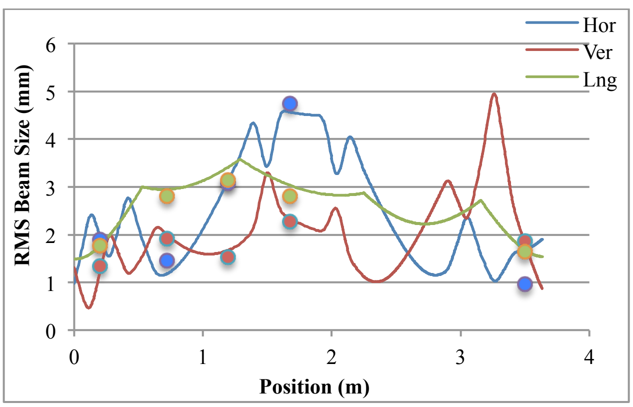

Figure 2: Continuation method solution.

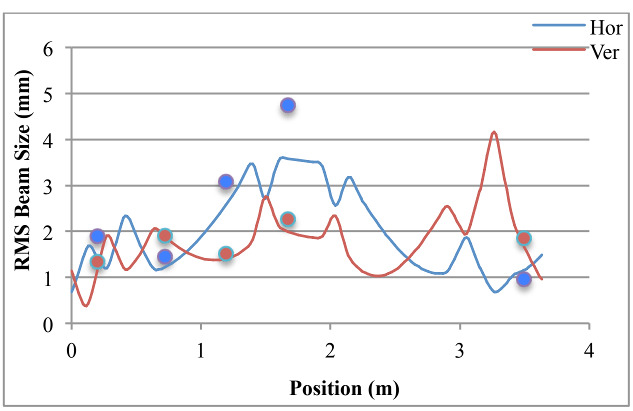

Figure 3: Data fitting solution.

Visual inspection suggests the fixed-point and continuation methods better reproduce the measurements than does data fitting. Indeed, referring to **Table 1** the error of data fitting is an order of magnitude larger. However, **Table 2** shows that error with the EMS-measured C-S parameters is smallest for the data fitting method. We are currently still resolving this conflict. Factors that may contribute are 1) profile and emittance measurement errors, 2) data post-processing, and 3) model errors. An additional possibility is a discrepancy in ion source beam current, affecting model accuracy.

Table 1: CS Parameters at EMS

Technique	Plane	Alpha	Beta	Emit	Res Err
Zero Chg	HOR	1.630	0.892	5.292	2.57e-6
	VER	-0.672	0.276	5.593	
Fixed-Pt	HOR	2.551	1.142	4.940	2.45e-6
	VER	-0.411	0.275	4.345	
Continue	HOR	2.061	0.927	5.472	5.18e-6
	VER	-0.551	0.276	4.634	
Data Fit	HOR	1.610	0.694	5.772	6.66e-4
	VER	-0.330	0.268	4.337	
Emit Scan	HOR	1.611	1.083	5.473	90%
	VER	0.126	0.312	4.668	95%

Table 2: Fractional Error from EMS Measurement

Plane	Zero Chg	Fxd-Pt	Contin	Data-Fit
HOR	0.1795	0.594	0.314	0.363
VER	4.339	4.264	5.374	3.623
TOTAL	4.343	4.305	5.383	3.641

CONCLUSIONS

Our ultimate objective is to automate accelerator matching using profile measurements. However, there are numerous difficulties in estimating the C-S parameters from beam size measurements. Techniques are necessarily model dependent and there are errors in the measurement, thus, any discrepancies are reflected in the answer. There is typically more data than parameters producing an over-determined system with no "true" solutions. However, the methods described here still have a well-defined solution. This is in contrast to a fully iterative technique where the solution is defined through a functional, which can have a significant (subjective) influence on the solution. In our example we are left with the ironic situation where the method with poorest merit produces the best predictive results. The cause of this situation is still being investigated.

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