The Nearest "Doubly Stochastic" Matrix to a Real Matrix with the same First Moment

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Let T be an arbitrary $n \times n$ matrix with real entries. We consider the set of all matrices with a given complex number as an eigenvalue, as well as being given the corresponding left and right eigenvectors. We find the closest matrix A, in Frobenius norm, in this set to the matrix T. The normal cone to a matrix in this set is also obtained. We then investigate the problem of determining the closest "doubly stochastic" (i.e. $A\mathbf{e} = \mathbf{e}$ and $\mathbf{e}^T A = \mathbf{e}^T$, but not necessarily nonnegative) matrix A to T, subject to the constraints $\mathbf{e}_1^T A^k \mathbf{e}_1 = \mathbf{e}_1^T T^k \mathbf{e}_1$, for $k = 1, 2, ...$ A complete solution is obtained via alternating projections on convex sets for the case $k = 1$, including when the matrix is nonnegative.

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1. Introduction

Let $\mathbf{e}$ be the $n \times 1$ vector of all ones, i.e. $\mathbf{e} = (1, 1, ..., 1)^T$, and let $\mathbf{e}_i$ denote the vector with a one in the ith position and zeros elsewhere. Let A be an $n \times n$ matrix with real entries, then we shall say that A is RC1 if $A\mathbf{e} = \mathbf{e}$ and $\mathbf{e}^T A = \mathbf{e}^T$ (A has row and column sums equal to one). If an RC1 matrix A also has each of its entries nonnegative then A is doubly stochastic (DS). A matrix which satisfies the first moment is said to be M_1, a nonnegative matrix is said to be NN.

Professor Zhaojun Bai suggested the following problem (whose application is described in the succeeding paragraph): Given a tridiagonal matrix T, how do you find the closest $RC1$ (not necessarily tridiagonal) matrix A to T, where you are also required to keep as many of the moments fixed as possible, i.e. $\mathbf{e}_1^T A^k \mathbf{e}_1 = \mathbf{e}_1^T T^k \mathbf{e}_1$, $k = 1, 2, ...$, for as many k values as possible.

The motivation for this problem arose from numerical simulation of large linear semiconductor circuit networks. In the model order reduction techniques for the approximation of the Laplace-domain transfer function of a linear network, a recent numerically stable algorithm is proposed for computing a Padé approximation using the Lanczos process [5]. The Lanczos process produces a tridiagonal matrix, which can be regarded as a low order approximation to the linear system matrix describing the large linear network. The tridiagonal matrix T is the best approximation in the sense of matching the maximal number of moments. Suppose the original system matrix is $RC1$, then the $n \times n$ tridiagonal matrix T is in general not $RC1$. We would like to find the closest $RC1$ $n \times n$ matrix A to T, and at the same time match the moments. We will not restrict ourselves to the case where T is tridiagonal.

Cheney and Goldstein [4] showed that alternating projections (to the respective nearest point) on two closed convex sets will converge to a point in the intersection, but not necessarily the nearest point to the given starting point. If the intersection is empty, the iterates converge to two points in the respective convex sets (oscillating between them), which are closest and give the distance between the sets. Boyle and Dykstra [3] (see also Gaffke and Mathar [6]) generalized the simple alternating projections with a modified algorithm which converges to the nearest point in the intersection (of a finite number of convex sets) to the original point. See [1] for a recent survey article.

In Section 2 we give an explicit form for the closest matrix, with a prescribed eigenvalue and corresponding right and left eigenvectors, to a given matrix. The $RC1$ matrices form a special case for this result. We determine, in Section 3, the normal cone to the set of these same matrices. Section 4 gives an algorithm (similar to the treatment in [7]) to find the closest $RC1$ matrix, with the same first moment as the given matrix T, including the nonnegative (doubly stochastic) case. Section 5 provides computational evidence of the algorithms effectiveness.

2. The closest $RC1$ matrix

We first derive a result which includes the $RC1$ matrices as a special case. Suppose the vectors $\mathbf{x}$, $\mathbf{y}$ and the complex number λ are given. We give an explicit form for the closest matrix A with right and left eigenvectors $\mathbf{x}$ and $\mathbf{y}$, corresponding to the eigenvalue λ, to a given matrix T. By "closest" we mean using the Frobenius norm $||X|| = \sqrt{\text{trace}(X^T X)}$ induced by the inner product $< X, Y >= \text{trace}(X^T Y)$. Observe that the set of matrices $K = \{Z \in \mathbf{R}^{n \times n} | Z\mathbf{x} = \lambda \mathbf{x},\ \mathbf{y}^T Z = \lambda \mathbf{y}^T\}$ is a convex set, i.e. given Z_1 and Z_2 in K, then for any $t \in [0, 1]$, it follows from the definition of K that $tZ_1 + (1 - t)Z_2 \in K$. Further, recall that for any point T outside a (closed) convex subset C of a Hilbert space there is a unique nearest point A in C to T [2].

To find the explicit form for the closest (in Frobenius norm) matrix A to a given matrix T, we minimize the function $f(T) = ||A - T||^2$ subject to the constraints $A\mathbf{x} = \lambda \mathbf{x}$

and $\mathbf{y}^T A = \lambda \mathbf{y}^T$.

The Kuhn-Tucker conditions yield

$$2(A - T) + 2\alpha\mathbf{x}^T + 2\mathbf{y}\beta^T = O,$$

where 2α and 2β are the vectors of Lagrange multipliers. We must now solve simultaneously the three equations $A = T - \alpha\mathbf{x}^T - \mathbf{y}\beta^T$, $A\mathbf{x} = \lambda\mathbf{x}$ and $\mathbf{y}^T A = \lambda\mathbf{y}^T$.

Substituting A into the latter two constraint equations above, and assuming without loss of generality that $||\mathbf{x}||_2 = ||\mathbf{y}||_2 = 1$, we are left with the problem of solving for $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ in the matrix equation

$$\begin{bmatrix} I & yx^T \\ xy^T & I \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} Tx - \lambda x \\ T^T y - \lambda y \end{bmatrix}.$$

It is easy to check (say, by calculating the characteristic polynomial using Schur complements) that the matrix $\begin{bmatrix} I & yx^T \\ xy^T & I \end{bmatrix}$ has $2(n-2)$ eigenvalues equal to 1, one eigenvalue equal to 2 and one eigenvalue equal to 0. We must find a particular solution $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ which produces the closest matrix A.

Multiplying both sides on the left by $\begin{bmatrix} I & -yx^T \\ -xy^T & I \end{bmatrix}$, we obtain a matrix equation which is easier to solve, namely

$$\begin{bmatrix} I - yy^T & O \\ O & I - xx^T \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} (I - yy^T)(Tx - \lambda x) \\ (I - xx^T)(T^T y - \lambda y^T) \end{bmatrix}.$$

This clearly has the general solution (note: the nullspace is now two dimensional)

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} Tx - \lambda x + \mu_1 y \\ T^T y - \lambda y + \mu_2 x \end{bmatrix},$$

for arbitrary μ_1 and μ_2.

After substituting this general solution into our original matrix equation, we find that we must also have $\mu_1 + \mu_2 + \mathbf{y}^T T\mathbf{x} - \lambda\mathbf{y}^T\mathbf{x} = 0$. Writing $\nu_1 = \mu_1 + (1/2)(\mathbf{y}^T T\mathbf{x} - \lambda\mathbf{y}^T\mathbf{x})$ and $\nu_2 = \mu_2 + (1/2)(\mathbf{y}^T T\mathbf{x} - \lambda\mathbf{y}^T\mathbf{x})$, so $\nu_1 + \nu_2 = 0$ or with $\nu = \nu_1 = -\nu_2$ we find that the general solution for our original matrix equation is

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} Tx - \lambda x - (1/2)(y^T Tx - \lambda y^T x)y \\ T^T y - \lambda y - (1/2)(y^T Tx - \lambda y^T x)x \end{bmatrix} + \nu \begin{bmatrix} y \\ -x \end{bmatrix}.$$

After substituting $\alpha = T\mathbf{x} - \lambda\mathbf{x} - (1/2)(\mathbf{y}^T T\mathbf{x} - \lambda\mathbf{y}^T\mathbf{x})\mathbf{y}$ and $\beta = T^T\mathbf{y} - \lambda\mathbf{y} - (1/2)(\mathbf{y}^T T\mathbf{x} - \lambda\mathbf{y}^T\mathbf{x})\mathbf{x}$ into $A = T - \alpha\mathbf{x}^T - \mathbf{y}\beta^T$ and rearranging we obtain

$$A = \lambda I + (I - \mathbf{y}\mathbf{y}^T)(T - \lambda I)(I - \mathbf{x}\mathbf{x}^T).$$

The following theorem shows that the matrix A is the nearest matrix, with left and right eigenvectors $\mathbf{x}$ and $\mathbf{y}$ and corresponding eigenvalue λ, to the given matrix T.

Theorem 2.1. *Let T be an $n \times n$ matrix with real entries. Let $\mathbf{x}$ and $\mathbf{y}$ be $n \times 1$ unit vectors with real entries and λ a complex number. Let $K = \{Z \in \mathbf{R}^{n\times n} | Z\mathbf{x} = \lambda\mathbf{x},\ \mathbf{y}^T Z = \lambda\mathbf{y}\}$. Then the matrix A given by*

$$A = \lambda I + (I - \mathbf{y}\mathbf{y}^T)(T - \lambda I)(I - \mathbf{x}\mathbf{x}^T)$$

is in K, and satisfies the requirement that $||T - A|| \leq ||T - Z||$ for all matrices Z in K.
Proof It is easy to check that $A\mathbf{x} = \lambda\mathbf{x}$ and $\mathbf{y}^T A = \lambda\mathbf{y}^T$. The near point of a convex set is characterized by requiring that ([6],[9])

$$< T - \text{near point}, Z - \text{near point} > \leq 0, \quad \text{for all } Z \in K. \qquad (1)$$

If Z is an arbitrary matrix in K we have

$$\begin{aligned} < T - A, Z - A > &=< T - \lambda I - (I - \mathbf{y}\mathbf{y}^T)(T - \lambda I)(I - \mathbf{x}\mathbf{x}^T), Z - A >, \\ &=< T - \lambda I, Z - A > - < (I - \mathbf{y}\mathbf{y}^T)(T - \lambda I)(I - \mathbf{x}\mathbf{x}^T), Z - A >, \\ &=< T - \lambda I, Z - A > - < T - \lambda I, (I - \mathbf{y}\mathbf{y}^T)(Z - A)(I - \mathbf{x}\mathbf{x}^T) >, \\ &=< T - \lambda I, Z - A > - < T - \lambda I, Z - A >, \end{aligned}$$

using the inner product properties $< UV, W >=< U, WV^T >=< V, U^T W >$ and the fact that $(I - \mathbf{y}\mathbf{y}^T)(Z - A)(I - \mathbf{x}\mathbf{x}^T) = Z - A$. We conclude that $< T - A, Z - A >= 0$, and that A is the desired nearest point.

Remark

The characterization in the inequality (1) above, showing that the matrix A is the nearest matrix in the given convex set (in Frobenius norm) to a given arbitrary matrix T, is well-known. Its usefulness may also be seen by deducing the nearest matrix $A = (a_{ij})$ to $T = (t_{ij})$ for the convex sets consisting of nonnegative matrices (take $a_{ij} = \max\{t_{ij}, 0\}$), symmetric nonnegative matrices (take $a_{ij} = \max\{(t_{ij} + t_{ji})/2, 0\}$), symmetric positive semidefinite matrices [8], etc.

Corollary 2.2. *Let T be an $n \times n$ matrix with real entries. Then the closest (in Frobenius norm) $RC1$ matrix to T is given by*

$$A = \frac{\mathbf{e}\mathbf{e}^T}{n} + T - \frac{1}{n}\mathbf{e}\mathbf{e}^T T - \frac{1}{n} T\mathbf{e}\mathbf{e}^T + \frac{\mathbf{e}^T T\mathbf{e}}{n^2}\mathbf{e}\mathbf{e}^T$$

Proof The set of $RC1$ matrices is $RC1 = \{Z \in \mathbf{R}^{n\times n} | Z\mathbf{e} = \mathbf{e},\ \mathbf{e}^T Z = \mathbf{e}^T\}$, thus the corollary follows from the theorem by taking $\lambda = 1$, $\mathbf{x} = \dfrac{\mathbf{e}}{\sqrt{n}}$ and $\mathbf{y} = \dfrac{\mathbf{e}}{\sqrt{n}}$.

3. Normal cones

Notice that the set of M_1 matrices, namely $M_1 = \{Z \in \mathbf{R}^{n\times n} | \mathbf{e}_1^T Z \mathbf{e}_1 = \mathbf{e}_1^T T \mathbf{e}_1\}$, is a closed convex set, as is the set of $RC1$ matrices, and the set of DS matrices. Let C be a convex set in $\mathbf{R}^n$ and $\mathbf{a} \in C$. The normal cone $N_C(\mathbf{a})$ [10] is defined as

$$N_C(\mathbf{a}) = \{\mathbf{y} \in \mathbf{R}^n | < \mathbf{y}, \mathbf{z} - \mathbf{a} > \leq 0 \text{ for all } \mathbf{z} \in C\}.$$

It is clear that for $A \in M_1$, since M_1 is an affine subspace (in fact a hyperplane), the normal cone to M_1 at A is $N_{M_1}(A) = \{\alpha \mathbf{e}_1 \mathbf{e}_1^T | \alpha \in \mathbf{R}\}$.

Theorem 3.1. *Let* $\mathbf{x}$ *and* $\mathbf{y}$ *be* $n \times 1$ *unit vectors with real entries, and* λ *a complex number. Let* $K = \{Z \in \mathbf{R}^{n\times n} | Z\mathbf{x} = \lambda \mathbf{x},\ \mathbf{y}^T Z = \lambda \mathbf{y}^T\}$*. Then if* $A \in K$ *the normal cone to* K *at* A *is given by*

$$N_K(A) = \{B \in \mathbf{R}^{n\times n} | B = \mathbf{y}\mathbf{a}^T + \mathbf{b}\mathbf{x}^T, \text{ where } \mathbf{a}, \mathbf{b} \in \mathbf{R}^n\}$$

Proof Rewriting the normal cone as

$$N_K(A) = \{\mathbf{T} - \mathbf{A} \in \mathbf{R}^{n\times n} | < T - A, Z - A > \leq 0, \text{ for all } Z \in K\},$$

we will determine all matrices $T - A$ where A is the near point in K corresponding to T.

We know from Theorem 2.1 that the expression $A = \lambda I + (I - \mathbf{y}\mathbf{y}^T)(T - \lambda I)(I - \mathbf{x}\mathbf{x}^T)$ gives the near point in K corresponding to T. Notice also that $A = \lambda I + (I - \mathbf{y}\mathbf{y}^T)(A - \lambda I)(I - \mathbf{x}\mathbf{x}^T)$. Subtracting these two formulas gives that

$$(I - \mathbf{y}\mathbf{y}^T)(T - A)(I - \mathbf{x}\mathbf{x}^T) = 0. \qquad (2)$$

Let Q_1 be the Householder matrix given by $Q_1 = I - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}$, where $\mathbf{v} = \mathbf{y} + \mathbf{e}_n$. Then Q_1 has the properties that $Q_1 Q_1 = I$, Q_1 is an orthogonal matrix and $Q_1 \mathbf{y} = -\mathbf{e}_n$. We also then have that $Q_1 \mathbf{y}\mathbf{y}^T Q_1 = \mathbf{e}_n \mathbf{e}_n^T$, and $Q_1(I - \mathbf{y}\mathbf{y}^T)Q_1 = I - \mathbf{e}_n \mathbf{e}_n^T$. Similarly, let $Q_2 = I - 2\frac{\mathbf{w}\mathbf{w}^T}{\mathbf{w}^T\mathbf{w}}$, where $\mathbf{w} = \mathbf{x} + \mathbf{e}_n$, then $Q_2(I - \mathbf{x}\mathbf{x}^T)Q_2 = I - \mathbf{e}_n\mathbf{e}_n^T$. Next, multiplying on the left of equation (2) by Q_1 and on the right of equation (2) by Q_2, we see that $Q_1(T - A)Q_2 = \begin{bmatrix} O & c_1 \\ c_2 & d \end{bmatrix}$, for some c_1, c_2 in $\mathbf{R}^{n-1}$ and $d \in \mathbf{R}$. Thus we conclude that the normal cone consists of matrices of the form

$$B = Q_1 \begin{bmatrix} O & c_2 \\ c_1 & d \end{bmatrix} Q_2 = Q_1(-\mathbf{e}_n\mathbf{a}^T - \mathbf{b}\mathbf{e}_n^T)Q_2 = \mathbf{y}\mathbf{a}^T + \mathbf{b}\mathbf{x}^T,$$

for some vectors $\mathbf{a}$, $\mathbf{b}$ in $\mathbf{R}^n$. This completes the proof.

Corollary 3.2. *Let* $A \in \mathbf{R}^{n\times n}$*. If* $A \in RC1$ *the normal cone to* $RC1$ *at* A *is given by*

$$N_{RC1}(A) = \{B \in \mathbf{R}^{n\times n} | B = \mathbf{e}\mathbf{a}^T + \mathbf{b}\mathbf{e}^T \text{ where } \mathbf{a}, \mathbf{b} \in \mathbf{R}^n\}.$$

Proof Follows from the theorem by taking $\lambda = 1$ and $\mathbf{x} = \mathbf{y} = \frac{\mathbf{e}}{\sqrt{n}}$.

4. $RC1$ and M_1

In this section we will describe the procedure by which, given a matrix T, we determine the closest (in Frobenius norm) matrix A which is both $RC1$ and satisfies the first moment, i.e. $A \in RC1 \cap M_1$. In order to find this closest matrix, we will employ the algorithm of Boyle and Dykstra. First, however, we will digress to show that $RC1 \cap M_1 \neq \emptyset$, which is an obvious necessary condition for convergence. In fact we do more than this, we show that there exist matrices which are $RC1$ and satisfy the first and second moments.

To establish some notation let us write the given $n \times n$ matrix T (the matrix which we want to approximate), in the form $T = \begin{bmatrix} t_{11} & a^T \\ b & S \end{bmatrix}$, where $t_{11} \in \mathbf{R}$, $\mathbf{a}$, $\mathbf{b} \in \mathbf{R}^{n-1}$, and $S \in \mathbf{R}^{(n-1)\times(n-1)}$, where $n \geq 2$. In this case the first and second moments are $\mathbf{e}_1^T T \mathbf{e}_1 = t_{11}$ and $\mathbf{e}_1^T T^2 \mathbf{e}_1 = t_{11}^2 + \mathbf{a}^T \mathbf{b}$.

If $n = 2$, there exist matrices which are $RC1$ and satisfy the first moment, but will in general not satisfy the second moment condition. To see this consider the matrix $\begin{bmatrix} t_{11} & 1-t_{11} \\ 1-t_{11} & t_{11} \end{bmatrix}$, which has its second moment completely determined.

If $n \geq 3$ and $t_{11} \neq 1$, take

$$\begin{bmatrix} t_{11} & \frac{a^T b}{1-t_{11}} & 0 & \cdots & 0 & \frac{(1-t_{11})^2 - a^T b}{1-t_{11}} \\ 1-t_{11} & & & & & \\ 0 & & & & & \\ \vdots & & & \ddots & & \\ 0 & & & & \ddots & \\ 0 & & & & & \end{bmatrix},$$

and if $n \geq 3$ and $t_{11} = 1$, take

$$\begin{bmatrix} 1 & (1/2)a^T b & -(1/2)a^T b & 0 & \cdots & 0 \\ 1 & \ddots & & & & \\ -1 & & & & & \\ 0 & & & & & \\ \vdots & & & & \ddots & \\ 0 & & & & & \end{bmatrix},$$

where in the first row and column the unspecified entries (represented by dots) are all zeros, and all other unspecified entries are arbitrary, since they do not affect the first and second moments, except that the row and column sums must be equal to 1. Hence there always exist matrices which are $RC1$ and satisfy the first and second moment constraints. We apply Boyle and Dykstra's alternating projections to find the nearest $RC1$ or doubly stochastic matrix with given first moment to a matrix T.

Let $M \in \mathbf{R}^{n\times n}$. Let $P_{RC1}(M)$ = closest $RC1$ matrix to M using Corollary 2.2; $P_1(M)$ = matrix M except that the $(1,1)$-entry is set equal to t_{11}; and P_{NN} = closest nonnegative matrix to M using the remark just before Corollary 2.2. Given $T \in \mathbf{R}^{n\times n}$ and a stopping criterion ϵ the following algorithm computes the nearest $X \in RC1 \cap M_1$ in Frobenius norm to T.

Algorithm 4.1 Set $A := T$.
For $i = 1, 2, 3, ...$ do
Set $B := P_{RC1}(A)$
Set $A := P_{M_1}(B)$
If $||A - B|| < \epsilon$ then stop.
Next i.

Since the set of $RC1$ matrices is a (closed) affine subspace, and the set of M_1 matrices is affine, and thus both sets are convex, so alternately projecting on these sets will produce the closest matrix in the intersection of these two sets, to the original matrix T, i.e. Boyle and Dykstra's algorithm is known to converge to the near point.

The following algorithm computes the nearest $X \in RC1 \cap M_1 \cap NN = DS \cap M_1$ in Frobenius norm to T. The last three steps, before the check for convergence are needed because the set of nonnegative matrices is convex, but not affine.

Algorithm 4.2 Set $A := T$, $Z := O$.
For $i = 1, 2, 3, ...$ do
Set $B := P_{RC1}(A)$
Set $C := P_{M_1}(B)$
Set $D := C - Z$
Set $E := P_{NN}(D)$
Set $A := E$
Set $Z := A - D$
If $||B - C|| < \epsilon$ and $||C - E|| < \epsilon$ and $||B - E|| < \epsilon$ then stop.
Next i.

5. Numerical experiments

In order to demonstrate the efficacy of our method, we provide three tables of data. In each of these tables we randomly generated twelve matrices T: four 100×100, four 250×250 and four 500×500. With these twelve matrices, we did the two cases $RC1 \cap M_1$ and $RC1 \cap DS$. Each row in the tables gives the average of the data for the four matrices of the given size. All computations were done on a Sun Ultra 1 using the gcc compiler.

"N" is the size of the matrices; "Time" is the cpu time in seconds required for convergence; "Its" gives the number of cycles through the projections required to satisfy the stopping criterion; "Sets" indicates which sets were projected onto, taken from $RC1$, M_1

and NN; "Dist" is the distance between T and the closest matrix A. Our stopping criterion for convergence was

$$||M\mathbf{e} - \mathbf{e}||_2 + ||M^T\mathbf{e} - \mathbf{e}||_2 + |\mathbf{e}_1^T M\mathbf{e}_1 - \mathbf{e}_1^T T\mathbf{e}_1| < 10^{-10}.$$

Table I

N	Time	Its	Sets	Dist
100	0.15	7	$RC1, M_1$	41.25
250	0.93	6	$RC1, M_1$	64.74
500	3.64	5	$RC1, M_1$	90.76

Table I contains the results of generating matrices $T = (t_{ij})$ with random entries uniformly distributed such that $-10 \leq t_{ij} \leq 10$, for $1 \leq i, j \leq n$. The convergence of the algorithm is as expected, since these are projections onto convex and affine sets.

Table II

N	Time	Its	Sets	Dist
100	46.95	1819	$RC1, NN, M_1$	287.53
250	359.77	1796	$RC1, NN, M_1$	720.82
500	1731.93	2007	$RC1, NN, M_1$	1441.86

For Table II we chose another twelve matrices T such that $-10 \leq t_{ij} \leq 10$, but we set $t_{11} = \frac{1}{2}$. This ensures that the intersection of the $RC1$, NN, and M_1 sets is nonempty.

Acknowledgements

The second author received partial support from National Science Foundation grant CHE-9005960. The third author received funding as a Postdoctoral Scholar from the Center for Computational Sciences, University of Kentucky.

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