

A kinematic investigation of the incorporation of constraints into
quantum optimal control: A report of the work done during the
summer of 2012

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As stated in my proposal for the PPST fellowship, a common goal of quantum control experiments is to achieve high quality manipulation of a quantum system by searching for an optimal control, typically drawn from the phases and amplitudes of an applied field. The search for an optimal field occurs on an underlying quantum control landscape, which is the observable as a function of the control field variables. Under certain assumptions the landscape will be free of suboptimal extrema that could prevent search algorithms from identifying optimal controls. However, one key landscape theory assumption is that no significant constraints are placed upon the control variables, and constraints on the controls will always be present in realistic laboratory settings. For example, the Ti: sapphire laser commonly used in quantum control experiments is centered at 800 nm with a 10 nm bandwidth, which restricts the pulses to only a limited wavelength range. The effect of restricting control resources on the ability to achieve optimal control is not well understood, and exploration of this topic is the subject of the research performed over the summer. The control variables presented are time-independent 'kinematic' controls, which act as a stand-in for dynamic controls, simplifying the Schrodinger equation-dependent dynamic controls into a different paradigm. By considering these kinematic control variables and how they behave when constrained and then mapping this kinematic control scheme to the traditional dynamic control scheme, we can use this simplified picture to understand how limiting resources affects the ability to achieve good control. We shall be trying to understand this kinematic control scheme with the problem of the unitary transformation scheme, wherein a unitary matrix U is transformed so as to retain its unitarity while attempting to bring it as close to possible to another unitary matrix W . Through simulations, the results can offer insight into constrained dynamic control and their optimal control capabilities.

In the traditional dynamic setting, and external control, denoted $\epsilon(t)$ and acting over a finite time interval $[0, T]$, consists of a large number of control variables such as amplitudes and phases. the internal energy of the quantum system may be described by the field-free Hamiltonian H_0 . The transition dipole μ dictates the strength of the permitted transitions upon interactions with the external field. We can simplify the quantum system, which is an infinite dimensional system, to a finite N -dimensional system, where H_0 and μ are $N \times N$ diagonal and Hermitian matrices, respectively. The time-dependent Hamiltonian that incorporates the external control $\epsilon(t)$ may then be written using the dipole approximation as:

$$H(t) = H_0 - \mu\epsilon(t) \tag{1}$$

and the dynamics of the system are represented by the time-dependent Schrodinger equation:

$$i\hbar\frac{\partial}{\partial t}U(t, 0) = H(t)U(t, 0), \quad U(0, 0) = \mathbb{1} \tag{2}$$

where $U(t,0)$ is a unitary propagator that solves the above equation and assumes the form:

$$U(t, 0) = \tau \exp\left(-\frac{i}{\hbar} \int_0^t H(t') dt'\right) \quad (3)$$

where τ represents the time-ordering operator. The observable we will use in the defining of this dynamic and kinematic approach to quantum control is that of the fidelity of the matrix U when compared to some matrix W , which is defined in a dynamic view as:

$$M(\epsilon(t)) = \|W - U(T, 0)\|^2 \quad (4)$$

where W is the target matrix we are trying to transform U into using the field $\epsilon(t)$ as the control variable. We evaluate the expression as the Frobenius norm, which means that the equation can be rewritten:

$$M(\epsilon(t)) = 2N - 2\text{Re}(\text{Tr}(W^\dagger U(T, 0))) \quad (5)$$

where N is the size of the matrix. The fact that local searches reach the optimal value for this observable is due to the lack of suboptimal critical points. This can be analytically proven and will now be summarized. A critical point of the $F(\epsilon(t))$ landscape corresponds to a point where:

$$\frac{\delta M}{\delta \epsilon(t)} = 0 \quad (6)$$

is true for all $0 \leq t \leq T$. The system is assumed to be controllable, meaning there exists a set of controls that yield any arbitrary observable value. In this formulation, the controls are also assumed to be unconstrained that they may assume any numerical value. To simplify the analysis of equation (6), we substitute the identity:

$$U = \exp(iA) \quad (7)$$

where A is an arbitrary $N \times N$ Hermitian matrix. This equality in (7) is the main feature of the kinematic model, substituting a time-independent formulation of U for the time-dependent dynamic formulation of U . We then can rewrite equation (5) as:

$$M(A) = 2N - 2\text{Re}(\text{Tr}(W^\dagger \exp(iA))) \quad (8)$$

This formulation of U is time-independent, so it subsumes the time-dependent Hamiltonian by setting the following equality as true:

$$\tau \exp\left(-\frac{i}{\hbar} \int_0^t H(t') dt'\right) = \exp(iA) \quad (9)$$

Now, we can expand equation (6) in terms of matrix elements of A to:

$$\frac{\delta M}{\delta \epsilon(t)} = \sum_{j,k} \frac{\delta M}{\delta A_{jk}} \frac{\delta A_{jk}}{\delta \epsilon(t)} = 0 \quad (10)$$

Since we are working under the assumption that the system is controllable, that implies that the functions $\frac{\delta A_{jk}}{\delta \epsilon(t)}$ are linearly independent, as any value of A_{pq} is reachable given the controllability of the system. This means that the following must be true:

$$\frac{\delta M}{\delta A_{jk}} = 0 \quad (11)$$

for all j, k , as $\frac{\delta A_{jk}}{\delta \epsilon(t)}$ cannot be 0, given controllability. An analysis of equation (11) shows that there exist critical points at $M = 0, 4, 8, \dots, 4N$, where 0 is where $U = W$, corresponding to perfect control, and where $4N$ is where $U = -W$. The rest of the critical points, upon further Hessian analysis, are saddle points, meaning that the only extrema on the landscape are where M is 0 or $4N$.

The above schema is both a much simpler way of analyzing the quantum control landscape and climbing the landscape, but also a valid set of controls. We recognize that there is a method of mapping the dynamic controls to the kinematic controls, which is from $\epsilon(t) \rightarrow A$, which is from many variables to few, and from kinematic controls back to dynamic controls, which is $A \rightarrow \epsilon(t)$, which is from few to many controls. This analysis of the mapping is important, especially from kinematic controls back to dynamic controls, as we can take the simple time-independent formulation of U and connect it to a physical field. One method by which we can convert dynamic to kinematic controls is to minimize the cost function:

$$J_{dk} = \|U(A) - U_{dyn}\|^2 \quad (12)$$

where we are dealing with the Frobenius norm again. By minimizing this over A , we get a mapping that brings the kinematically defined U , where U is created by solving for A , as close as possible to the dynamically defined U , through H_0 , μ , and $\epsilon(t)$. Conversely, the mapping from kinematic to dynamic controls occurs through the minimization of

$$J_{kd} = \|U_{kin} - U(H(t))\|^2 \quad (13)$$

over $H(t)$, where $U(H(t))$ is the dynamically defined unitary matrix. This mapping is important because a constrained kinematic control that has been analyzed and understood can be mapped to a constrained dynamic control, which is harder to understand than the constrained kinematic control.

Resources are always constrained in some manner. For example, laser pulses in quantum control experiments are constrained to some operational frequency and limited bandwidth. Thus, we wish to understand more deeply the effect of constraints upon quantum control. The first step to generalizing the impact

of these constraints is to utilize kinematic controls with the knowledge that the results can be mapped to a dynamic scenario. The kinematic controls enable a variety of constraints to be considered that not only reflect external field controls but also constrains of the quantum system itself.

Before introducing the method developed to vary kinematic controls to extremize an observable subject to constraints, it is worthwhile to examine particular constraint functions that can be considered. In dynamics, an important control resource is the control pulse energy or fluence:

$$F_{dyn} = \int_0^T \epsilon^2(t), dt \quad (14)$$

When pulse phases are treated as control variables, the fluence remains constant, as changing the phase of the pulse will not change the amplitude of the pulse, which is what the energy of the pulse will be dependent upon. The internal energy of the system and the allowed state transitions, represented by the matrices H_0 and μ , respectively, are assumed to remain constant. In the kinematic picture, since we subsume $\epsilon(t)$ into the A matrix formulation, we can define the kinematic fluence as:

$$F = \text{tr}(A^\dagger A) \quad (15)$$

We may also limit what state-to-state transitions are accessible during optimization, which entails fixing the corresponding A matrix elements. This is analogous to allowing only specific transitions by changing the transition dipole matrix μ in both the W and the $P_{i \rightarrow f}$ problem. Another constraint that may arise in a physical system is that of the bandwidth. For example, for a Ti:Sapphire laser centered at 800 nm has a bandwidth of $\Delta\lambda \approx 10\text{nm}$, which represents an important constraint. The kinematic definition of the bandwidth can be written as:

$$L = \left[\frac{\sum_{j,k} A_{jk}^2 (j-k)^2}{\sum_{j,k} A_{jk}^2} \right]^{\frac{1}{2}} \quad (16)$$

This can be thought of as addressing the combined strength of the available transitions, as in what transitions are most favorable. We now address the mathematics developed to incorporate these or other constraints into kinematic optimization.

To explore the kinematic landscape, we want to use a local gradient-based algorithm called D-MORPH, which utilizes small diffeomorphic changes to optimize a set of controls. The diffeomorphic parameter s is used such that $A \rightarrow A(s)$ so as to ensure a smooth, continuous trajectory on the landscape. The controls that we are going to be analyzing will be the elements of A , where the elements will be denoted by the index markers p and q , which indicate what element of A we are analyzing, so each element will be some A_{pq} . Since, to have the observable M laid out in equation (8) be monotonically decreasing so as to reach optimal control of $M = 0$, we want to have $\frac{dM}{ds} \leq 0$, which, upon utilizing the chain rule, can also be

written:

$$\frac{\partial M(U)}{\partial s} = \sum_{pq} \frac{\partial M(U)}{\partial A_{pq}} \frac{\partial A_{pq}}{\partial s} \leq 0 \quad (17)$$

And we are trying to derive an expression for $\frac{\partial F(U)}{\partial A_{pq}}$. To do so, we consider that, without any constraints placed upon the available controls, monotonic decrease of the observable M will occur if the following condition is met:

$$\frac{dA_{pq}}{ds} = -\beta_{pq} \frac{\partial M}{\partial A_{pq}} \quad \beta_{pq} > 0 \quad (18)$$

For all pq . Now, we want to try to evaluate $\frac{\partial M(U)}{\partial A_{pq}}$ using our definition of M from equation (8). First, we write that:

$$\frac{\partial M(U)}{\partial A_{pq}} = -2 \frac{\partial}{\partial A_{pq}} \text{Tr}[\text{Re}(W^\dagger U)] \quad (19)$$

The $2N$ disappears because it is a constant and not dependent upon the elements of A . We can bring the derivative inside the Trace and real functions and also consider the fact that W can be defined as $W = e^{iB}$ where B is a matrix that is just like A , and this shows us that B is not dependent upon A . Now, we see that (19) is:

$$\frac{\partial M(U)}{\partial A_{pq}} = -2 \text{Tr}[\text{Re}(W^\dagger \frac{\partial U}{\partial A_{pq}})] \quad (20)$$

Since $U = e^{iA}$, we can rewrite (20) using the identity:

$$\frac{\partial e^{iA}}{\partial A_{pq}} = i \int_0^1 e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj \quad (21)$$

and get that:

$$\frac{\partial M(U)}{\partial A_{pq}} = -2 \text{Tr}[\text{Re}(W^\dagger i \int_0^1 e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj)] \quad (22)$$

Now, in equation (22), since W^\dagger is not dependent upon j , we can rewrite (22) using $W^\dagger = e^{-iB}$. Also, considering the fact that:

$$\text{Re}(iZ) = \text{Re}(ia - b) \quad (23)$$

$$= -b \quad (24)$$

$$= -\text{Im}(Z) \quad (25)$$

Therefore, we have:

$$\frac{\partial M(U)}{\partial A_{pq}} = -2\text{Tr}[\text{Re}(i \int_0^1 e^{-iB} e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj)] \quad (26)$$

$$= 2\text{Tr}[\text{Im}(\int_0^1 e^{-iB} e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj)] \quad (27)$$

Since we assume we know what matrix B is, as that is our target matrix to be able to create W, this equation is only dependent upon our variations in the elements of A, so we have obtained our formulation for $\frac{\partial F(U)}{\partial A_{pq}}$ and using that in equation (18) with all $\beta_{pq} = 1$ then we get:

$$\frac{dA_{pq}}{ds} = -2\text{Tr}[\text{Im}(\int_0^1 e^{-iB} e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj)] \quad (28)$$

which can be solved to obtain a control trajectory for the elements of A that will yield a monotonic decrease.

Now, we can use this D-MORPH technique if constraints are to be imposed during optimization. To simultaneously satisfy multiple constraints, we define a constraint column vector $C(A_{pq})$ that is defined as $C = [C_1, C_2, \dots, C_Q] = 0$, which contains Q distinct constraints that are set equal to 0. To simultaneously maintain $C = 0$ while decreasing M requires ensuring that:

$$\frac{dC_q}{ds} = 0 \quad (29)$$

for all $q = 1, \dots, Q$. while also satisfying equation (17). We can expand equation (29) in terms of the A_{pq} , which will yield:

$$\frac{dC_q}{ds} = \sum_{p,q} \frac{\partial C_q}{\partial A_{pq}} \frac{dA_{pq}}{ds} = 0 \quad (30)$$

Now, we may have $\frac{\partial C_q}{\partial A_{pq}}$ be a matrix element of an $S \times Q$ matrix Ω where each column corresponds to the length- S gradient vector of a particular constraint C_q . S is equivalent to N^2 here. To satisfy equation (30), we can introduce a projector $P(s)$ that fulfills the following:

$$\frac{dA_{pq}}{ds} = P(s)f(s) \quad (31)$$

where $P(s)$ is an $S \times S$ positive semi-definite projector defined as:

$$P(s) = \mathbb{1} - \Omega(s)(\Omega^\top(s)\Omega(s))^{-1}\Omega^\top(s) \quad (32)$$

where \top denotes the matrix transpose and $f(s)$ can be any length- S vector. By substituting equation (31) into equation (17), we will get:

$$\frac{\partial M(U)}{\partial s} = \left(\frac{\partial M(U)}{\partial A_{pq}} \right)^\top P(s) f(s) \quad (33)$$

and if set:

$$f(s) = -\frac{\partial M(U)}{\partial A_{pq}} \quad (34)$$

that will ensure that (33) will be monotonically decreasing while fulfilling the Q constraint functions that have been implemented.

A concrete example of this constrained D-MORPH algorithm is that of the fixed fluence constraint. If we consider a certain system in which the initial fluence of a real symmetric matrix A is F_0 and the goal is to minimize W while maintaining the following:

$$F - F_0 = 0 \quad (35)$$

then we must satisfy the condition that:

$$\frac{dF}{ds} = \sum_{m=1}^M \frac{\partial F}{\partial A_{pq}} \frac{dA_{pq}}{ds} = 0 \quad (36)$$

which can be maintained as such if:

$$\frac{\partial F}{\partial A_{pq}} = 2\text{Tr}\left(A \frac{\partial A}{\partial A_{pq}}\right) \quad (37)$$

We can then utilize the general constraint formulation detailed previously with Ω , which is the $S \times 1$ gradient vector $\frac{\partial F}{\partial A_{pq}}$, which is used to produce the projector P as defined in equation (32) and write what $\frac{dA_{pq}}{ds}$ is, which is:

$$\frac{dA_{pq}}{ds} = -P \frac{dM}{dA_{pq}} \quad (38)$$

which produces both a decrease in the value of M and satisfies the fixed fluence constraint.

To be able to create a mapping from the kinematic to the dynamic picture, we now lay out a procedure to do so. When using kinematic controls in this unitary transformation problem, optimization yields sets of kinematic matrices A with corresponding M values. The D-MORPH procedure that had been laid out elsewhere can be thought of as utilizing the diffeomorphic variable s as an iteration index, such that for each s , there exists a corresponding N -dimensional $A(s)$, an M value, and another N -dimensional $U(s) = \exp(iA(s))$. The first step in the mapping between kinematic and dynamic models is to identify the

dynamic parameters H_0 and μ as well as external field $\epsilon(t)$ that produce the initial $U(s = 0)$. The choosing of these parameters should of course create a whole dynamically defined U matrix that matches the kinematic U matrix. For the mapping to be both meaningful and easier, it is imperative that the parameters of H_0 and μ relate in some way to A structurally. Even with carefully constructed structural parameters, the chances of choosing a field $\epsilon(t)$ that maps those to elements to a kinematic U is virtually 0, so we take our defined H_0 and μ values and perform an optimization where we search for the appropriate $\epsilon(t)$. To do so, we can minimize the cost function J_{kd} where:

$$J_{kd}(s = 0) = \|U(s = 0) - U(H_0, \mu, \epsilon(t))\|^2 \quad (39)$$

Upon optimization, where $U(H_0, \mu, \epsilon(t))$ and $U(s = 0)$ are arbitrarily close, we then perform the same optimization for $U(s = 1)$ and onwards over all of $U(s)$. This will create a dynamic trajectory for the problem. The next part of this summary includes some of the data that was collected this summer while laying out further tests that can be run.

Two methods of analyzing the W problem that could provide numerical insight into what happens with introduction of constraints into quantum control is that of the fixed variable case and the fixed fluence case, which were detailed earlier. The fixed fluence tests have not performed yet, but I performed and analyzed the data on the fixed variable case. In this case, we utilized the equation laid out in (5) with an additional factor of $\frac{1}{4N}$ multiplied against the equation in (5) so as to normalize the values of M . In this experiment, I randomly chose one element in A and fixed it while allowing all the other elements to vary so as to try to minimize M . The results of this experiment for dimension $N = 2$ to dimension $N = 9$ are shown as follows:

Dimension	Mean Initial M	Mean Final M	Upper Deviation	Lower Deviation	Number of Data Points
2	.171259	.065909863	.121955985	.0522335511	100
3	.202345	.032635216	.048635091	.024051829	100
4	.244387	.009009863	.019769414	.007138511	100
5	.279182292	.003599763	.018578783	.002987605	96
6	.294838889	.001322288	.011378964	.001055606	90
7	.337210769	.00099077	.002879053	.000773067	65
8	.3623	.001369966	.002788328	.001009356	50
9	.367952632	.001518018	.003026978	.001210953	38

Table 1: Table of Relevant Compiled Means and Deviations

The expected behavior was shown, with M going down as dimension increased until we got to di-

mensions $N = 8$ and $N = 9$. So, I ran the tests again for the higher dimensions to see if it happened again and obtained these results:

Dimension	Mean Initial M	Mean Final M	Upper Deviation	Lower Deviation
7	.337	.00113	.00429	.000849
8	.352	.00153	.00268	.00121
9	.389	.00291	.00425	.00208
10	.399	.00102	.00450	.000733

Table 2: Table of Relevant Compiled Means and Deviations

In this experiment, as before, the showed results that were not the expected behavior. After testing to see if there was any error in the integrator, this anomaly was set aside for further consideration in lieu of doing other things this summer.

Another case that might be of interest is the bounded fluence case, in which, rather than the fluence only staying at a certain number, it may vary as long as it stays below a certain value. This also has yet to be done but will be performed in the future.

Another case that does not involve kinematics exactly but is still useful in defining and analyzing the W problem is that of the multiplicative update definition of the U matrix. This has the U matrix defined as, rather than $U = e^{iA}$, either $U = e^{iA}U_0$ or $U = e^{iA}U_0e^{iA}$, where U_0 is some initial unitary matrix. The former definition has been analyzed and does not work as the unconstrained formulation is not able to take some starting matrix U and have it converge to W every time, as the definition causes a loss of symmetric-ness within a few iterations and thus has difficulty converging to a symmetric W matrix with any sort of effectiveness. The latter definition will be derived analytically and investigated numerically in the future, but since I have yet to do it, I will not include it here. It does hold more hope to be effective, as the update step should maintain the symmetric-ness of U . Also, it is not actually a kinematic definition of the problem, another reason not to have it, but it could provide numerical insights into the W problem while being much much faster than the current formulation, so I believe it is worth mentioning. One other method of examining the W problem that will be explored in the future using kinematic definitions I will outline as follows:

We have defined our U matrix as e^{iA} and our W matrix as some fixed e^{iB} , where B is also real and symmetric. Rather than trying to have complete fidelity, having the U matrix match the W matrix exactly, we can try to match a smaller portion of the matrix. For example, if U is some symmetric matrix where the

entries are complex:

$$\begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix} \quad (40)$$

and W is some symmetric matrix where the entries are complex:

$$\begin{pmatrix} g & h & i \\ h & j & k \\ i & k & l \end{pmatrix} \quad (41)$$

rather than trying to have U be equal to W , we can have some smaller submatrix of U , such as:

$$U_{sub} = \begin{pmatrix} a & b \\ b & d \\ c & e \end{pmatrix} \quad (42)$$

be equal to the corresponding submatrix of W :

$$W_{sub} = \begin{pmatrix} g & h \\ h & j \\ i & k \end{pmatrix} \quad (43)$$

While maintaining unitarity of the whole U and W matrices. To measure the distance between the corresponding submatrices, we want to define the following equation,:

$$M_{sub}(U_{sub}) = ||W_{sub} - U_{sub}||^2 \quad (44)$$

Where U_{sub} is the U submatrix and W_{sub} is the W submatrix. This equation can be rewritten, for an $E \times K$ submatrix, where $E \leq N$ and $K \leq N$:

$$M_{sub}(U_{sub}) = 2K - 2\text{Re}(\text{Tr}(W_{sub}^\dagger U_{sub})) \quad (45)$$

Since we want the following to be true:

$$\frac{dM_{sub}}{ds} = \frac{dM_{sub}}{dA_{pq}} \frac{dA_{pq}}{ds} \leq 0 \quad (46)$$

for all p, q so that the value of M_{sub} is monotonically decreasing, we want the equation:

$$\frac{dA_{pq}}{ds} = -\frac{dM_{sub}}{dA_{pq}} \quad (47)$$

to be true. We can rewrite U_{sub} as ZUX , where Z and X are some matrices such that:

$$U_{sub} = ZUX \quad (48)$$

and U is e^{iA} , an $N \times N$ matrix. This makes Z an $E \times N$ matrix and X an $N \times K$ matrix. Now, when we apply $\frac{d}{dA_{pq}}$ to M_{sub} so as to get $\frac{dA_{pq}}{ds}$, we will get:

$$\frac{dM_{sub}}{dA_{pq}} = -2 \frac{d}{dA_{pq}} \text{Re}(\text{Tr}(W_{sub}^\dagger U_{sub})) \quad (49)$$

$$= -2 \text{Re}(\text{Tr}(W_{sub}^\dagger (Z \frac{dU}{dA_{pq}} X))) \quad (50)$$

$$= -2 \text{Re}(\text{Tr}(W_{sub}^\dagger (Z \frac{de^{iA}}{dA_{pq}} X))) \quad (51)$$

$$= 2 \text{Im}(\text{Tr}(W_{sub}^\dagger (Z \int_0^1 e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj X))) \quad (52)$$

Which makes $\frac{dA_{pq}}{ds}$ from equation (47)

$$\frac{dA_{pq}}{ds} = -2 \text{Im}(\text{Tr}(W_{sub}^\dagger (Z \int_0^1 e^{iA(1-j)} \frac{\partial A}{\partial A_{pq}} e^{iAj} dj X))) \quad (53)$$

Solving for this should yield the submatrices being close together without placing a restriction on the rest of the matrix. This derivation allows for update of the whole A matrix while only trying to make U_{sub} and W_{sub} close together. Since A remains symmetric, then U has to remain unitary, as $e^{iA}(e^{iA})^\dagger$ will be $\mathbb{1}$ for all symmetric A matrices. And I believe that U only has to remain unitary on the whole, as picking as a submatrix some rectangular matrix such as we did with U_{sub} in equation (42) makes it impossible to achieve unitarity for the submatrix as matrices can only be unitary when they are square. I believe this is a possible formulation of the problem, though possible problems arise in how to properly choose the entries of Z and X . Simulations will have to be run to see if those matrices can be chosen arbitrarily or if those matrices must have certain characteristics.

In all, this summer's work yielded some interesting results and has opened up new avenues of research, such as the investigation into why the values of M didn't behave as expected when the dimension N increases, as well as the various kinds of other constraints that can be used to investigate the effects of constraints upon this W problem.