Expressing linear equality constraints in feedforward neural networks

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Abstract

We seek to impose linear, equality constraints in feedforward neural networks. As top layer predictors are usually nonlinear, this is a difficult task if we wish to use standard convex optimization methods and strong duality. To overcome this, we introduce a new saddle-point Lagrangian with auxiliary predictor variables on which constraints are imposed. Eliminating the auxiliary variables leads to a dual minimization problem on the Lagrange multipliers introduced to satisfy the linear constraints. This minimization problem is combined with the standard learning problem on the weight matrices. From this theoretical line of development, we obtain the surprising interpretation of Lagrange parameters as additional, penalty layer hidden units with fixed weights stemming from the constraints. Consequently, standard minimization approaches can be used despite the inclusion of Lagrange parameters—a very satisfying, albeit unexpected, discovery.

1 Introduction

The current resurgence of interest and excitement in neural networks, mainly driven by high performance computing, has tended to shift the research focus away from applied math development. While this has enabled a dizzying array of practical applications and has firmly brought artificial intelligence and machine learning into the mainstream, fundamental issues remain. One such issue is the enforcement of constraints in neural network information processing. By far the most common architecture is the feedforward neural network with its implicit hidden units, nonlinearities and divergence measures linking predictors to targets. However, if we seek to impose mathematically specified constraints on the predictors since the targets satisfy them, there is a paucity in the literature to address this issue. A survey of the literature brings out methods that softly impose constraints using penalty functions and there is a smattering of work focused on constraint satisfaction, but in the main, there is no work that makes the satisfaction of hard equality constraints central to its mission. Addressing this lack is the motivation behind the paper.

The principal difficulty in imposing linear (or other) equality constraints lies in the nonlinear nature of the predictor of the output. In a standard feedforward network, the predictor is often a pointwise nonlinearity applied to a linear transformation of the output of the penultimate layer. Enforcing linear constraints on the predictor using standard Lagrangian methods is not straightforward as they effectively result in a set of nonlinear constraints on the top layer weights—difficult therefore (at first glance) to cast using standard convex optimization methods. Not taking advantage of convex optimization and duality would be unfortunate given the richness (and simplicity) of the methods at hand. On the other hand, the softmax nonlinearity is a clear cut example of a hard (sum to one) constraint being enforced, usually at the top layer to obtain one-of-$K$ multi-class soft memberships. This seems to run counter to our argument that enforcing constraints on nonlinear predictors is difficult. We therefore ask (and answer in the affirmative) the following question: can this example be generalized to other constraints?

We show that linear equality constraints can be expressed in feedforward neural networks using standard convex optimization methods. To achieve this, we introduce auxiliary variables (one set for each training set instance) and express the constraints on them. It turns out that we obtain a maximization problem on
the auxiliary variables (which take the form of predictors) and even more crucially, we obtain a convex dual minimization problem on the Lagrange parameter vectors upon elimination of the auxiliary set. Furthermore, if the form of the output nonlinearity is carefully matched with the choice of the output divergence measure, the Lagrange parameters can be interpreted as additional penultimate layer hidden units which connect to the output via fixed weights (depending on the constraints). This is a crucial discovery since these additional variables can be coupled by standard means to lower layers (finding application in compression autoencoders for example). No saddle-point methods are needed and while it may be necessary to explicitly solve for the Lagrange parameters in certain applications, we can deploy standard stochastic gradient descent methods here—a huge computational advantage.

The development of the basic idea proceeds as follows. We begin with the multi-class logistic regression (MC-LR) negative log-likelihood (which can serve as the top layer) and note (as mentioned above) that the softmax nonlinearity of the predictor satisfies a sum to one constraint. Then, we use an Ansatz (an educated guess) for the form of the saddle-point Lagrangian parameter with auxiliary variables, which when eliminated results in a dual minimization on the Lagrange parameter used to set up the softmax one-of-$K$ membership constraint. Subsequently, we show that a difference between squared $\ell_2$ norms can serve as a principle for setting up a saddle-point Lagrangian with linear constraints—albeit one with a linear output layer. Moving forward to discover a principle, the next step in the technical development is crucial: we identify the difference of squared $\ell_2$ norms as a special case of the difference of Bregman divergences with a direct relationship between the choice of the output nonlinearity and the form of the Bregman divergence [Bregman, 1967]. Once this identification has been made, the remainder of the development is entirely straightforward. Auxiliary variables (arranged in the form of predictors) are eliminated from the difference of Bregman divergences saddle-point Lagrangian leaving behind a dual minimization w.r.t. the Lagrange parameter vectors while continuing to obtain a standard minimization problem w.r.t. the network weights. Matching the nonlinearity to the choice of the Bregman divergence is important and we further require the output nonlinearity to be continuous, differentiable and monotonic. Provided these conditions are met, we obtain penultimate layer hidden unit semantics for the Lagrange parameters—a surprising (but obvious in hindsight) result.

2 A summary of the constraint satisfaction approach

We present a very brief summary of the basic result. Assume a feedforward neural network wherein we have the situation that the targets $\{y_n\}_{n=1}^N$ with $y_n \in \mathbb{R}^K$ satisfy the constraints $Ay_n = b_n$ where $b_n \in \mathbb{R}^I$. Here the matrix of constraint weights $A \equiv [a_1, \ldots, a_K]$. We would therefore like the nonlinear predictor from the top layer of the network also satisfy (or approximately satisfy) these constraints. Assume top layer weights $W \equiv [w_1, \ldots, w_K]$ and penultimate layer hidden units $x \in \mathbb{R}^J$. (It should be clear that $K > I$ and that usually $J > K$.) Then, consider the following loss function of the neural network (written in terms of the top layer weights and for penultimate layer hidden units and for a single instance):

$$\ell(W, \lambda) = -y^T(W^T x + A^T \lambda) + e^T \phi(W^T x + A^T \lambda)$$

(1)

where $e$ is the vector of all ones, $\lambda \in \mathbb{R}^I$ and $\phi$ is a vector of convex, differentiable functions $\phi(u) \equiv [\phi(x_1), \ldots, \phi(x_K)]^T$. We assume the output nonlinearity corresponding to the nonlinear predictor is pointwise and chosen to be $z = \sigma(u) \equiv \phi'(u)$.

We now minimize the loss function w.r.t. $\lambda$ in (1) by differentiating and setting the result to the origin to get

$$\nabla_\lambda \ell(W, \lambda) = -Ay + Az = 0 \Rightarrow -b + Az = 0$$

(2)

where $z = [\phi'(w_1^T x + a_1^T \lambda), \ldots, \phi'(w_K^T x + a_K^T \lambda)]^T$. This implies that the loss function in (1) is an objective function w.r.t. $\lambda$ as well as the weights of the feedforward neural network. Furthermore, there exists one $\lambda$ vector per input instance and when we minimize the loss function w.r.t. $\lambda$, we obtain a nonlinear predictor
z which satisfies the output constraints $A z = b$. The price of admission therefore is an additional set of $\lambda$ units (with fixed weights $A$) which need to be updated in each epoch. In the rest of the paper, we develop the theory underlying the above loss function.

3 Formal development of saddle-point Lagrangians and their dual

3.1 The Multi-class Logistic Regression (MC-LR) Lagrangian

The negative log-likelihood for multi-class logistic regression is

$$- \log \Pr(Y = y|W, x) = - \sum_{k=1}^{K} y_k w_k^T x + \log \sum_{k=1}^{K} \exp \{w_k^T x\}$$

(3)

where the weight matrix $W$ comprises a set of weight vectors $W = [w_1, \ldots, w_K]$, the class label column vector $y = [y_1, \ldots, y_K]^T$ and the log-likelihood is expressed for a generic input-output training set pair $(x, y)$.

Rather than immediately embark on a tedious formal exposition of the basic idea, we try and provide in- tuition. We begin with an Ansatz (an informed guess based on a result shown in [Yuille and Kosowsky, 1994]) that leads to (3) and then provide a justification for that educated guess. Consider the following Lagrangian Ansatz for multi-class logistic regression:

$$L_{MC-LR}^{(total)}(W, \{z_n\}, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ (z_n - y_n)^T W^T x_n - e^T \psi(z_n) + \lambda_n \left(e^T z_n - 1\right) \right]$$

$$= \sum_{n=1}^{N} \left[ (z_{nk} - y_{nk}) \sum_j w_{jk} x_{nj} - \sum_k \psi(z_{nk}) + \lambda_n \left(\sum_k z_{nk} - 1\right) \right]$$

(4)

where $z = [z_1, \ldots, z_K]^T$ is the auxiliary variable predictor of the output, $\psi(z) \equiv [\psi(z_1), \ldots, \psi(z_K)]^T$ is the negative entropy and $e$ is the column vector of all ones with

$$\psi(z) = z \log z - z. \tag{5}$$

(We use the term negative entropy for $\psi$ since it returns the negative of the Shannon entropy for the standard sigmoid.) The one-of-$K$ encoding constraint is expressed by a Lagrange parameter $\lambda$ (one per training set instance). In the context of the rest of the paper, the specific nonlinearity (in place of the sigmoid nonlinearity) used for MC-LR is $\sigma(u) \equiv \exp \{u\}$, its indefinite integral—the sigmoid integral—$\phi(u) \equiv \exp \{u\}$, the inverse sigmoid $u(z) \equiv \sigma^{-1}(z) = (\phi)^{-1}(z) = \log z$ and the negative entropy $\psi(z) \equiv z(u(z) - \phi(u(z)) = z \log z - z$ (effectively a Legendre transform of $\phi(u)$ [Legendre, 1787] [Mjolsness and Garrett, 1990]). The notation used in (4) and in the rest of the paper is now described.

Notation:

$\sigma(u), \phi(u), u(z)$ and $\psi(z)$ are the generalized sigmoid, sigmoid integral, inverse sigmoid and negative entropy respectively and correspond to individual variables ($u$ and $z$ both in $\mathbb{R}$). Please see Table 1 for examples. Boldfaced quantities always correspond to vectors and/or vector functions as the case may be. For example, $\sigma(u)$ is not a tensor and is instead unpacked as a vector of functions $[\sigma(u_1), \ldots, \sigma(u_K)]^T$. The same applies for $u(z)$, $\phi(u(z))$ and $\psi(z)$. Likewise, $\nabla \psi(v)$ is not a gradient tensor but refers to the vector of derivatives $[\psi'(v_1), \ldots, \psi'(v_K)]^T$. $e$ is the vector of all ones with implied dimensionality. Similarly, $\nabla u(z)$ is a vector of derivatives $[u'(z_1), \ldots, u'(z_K)]^T$ and $z \circ \nabla u(z)$ is a vector with $\circ$ denoting component-wise multiplication, i.e. $[z_1 u'(z_1), \ldots, z_K u'(z_K)]^T$. In an identical fashion, $\nabla_u \phi(u(z))$ is a vector of derivatives $[\phi'(u(z_1)), \ldots, \phi'(u(z_K))]^T$ and $\nabla \phi(u(z)) \circ \nabla u(z)$ denotes the vector formed by component-wise multiplication $[\phi'(u(z_1)) u'(z_1), \ldots, \phi'(u(z_K)) u'(z_K)]^T$. The Bregman divergence $B(z||v) \equiv \sum_{k=1}^{K} B(z_k||v_k)$—the sum of component-wise Bregman divergences. Uppercase variables (such as $W, A$) denote matrices with entries $\{w_{kj}\}$ and $\{a_{ki}\}$ respectively and $O$ denotes the origin. Lagrangian notation $L$ is strictly reserved for (optimization or saddle-point) problems with constraints. Individual training set instance pairs $(x, y)$ are often referred to with the instance subscript index $n$ suppressed.
| Name | Expression $\sigma(u)$ | Sigmoid integral $\phi(u)$ | Inverse sigmoid $u(z)$ | Negative entropy $\psi(z)$ | Bregman divergence $B(z|v)$ |
|------|-----------------|-----------------|-------------------|-----------------|-----------------|
| exp  | $\exp\{u\}$    | $\exp\{u\}$    | $\log z$          | $z \log z - z$ | $z \log z - z + v$ |
| sig  | $\frac{1}{1 + \exp(-u)}$ | $\log (1 + \exp\{u\})$ | $\frac{1}{1 - z}$ | $z \log z + (1 - z) \log(1 - z)$ | $z \log \frac{z}{1 - z} + (1 - z) \log \frac{1 - z}{z}$ |
| tanh | $\tanh u$       | $\log \cosh u$  | $\frac{1}{2} \log \frac{1 + z}{1 - z}$ | $\frac{1}{2} \log(1 + z) + \frac{1}{2} \log(1 - z)$ | $\frac{1}{2} \log \frac{1 + z}{1 - z} + \frac{1}{2} \log \frac{1 - z}{z}$ |
| SRLU | $\frac{a u \exp\left[\frac{u^2}{2}\right] + b u \exp\left[\frac{bu^2}{2}\right]}{\exp\left[\frac{u^2}{2}\right] + \exp\left[\frac{bu^2}{2}\right]}$ | $\log \left( \exp\left\{\frac{au^2}{2}\right\} + \exp\left\{\frac{bu^2}{2}\right\} \right)$ | $\frac{1}{2}$ | $-$ | $-$ |

Table 1: Generalized sigmoid to Bregman divergence table. SRLU stands for soft rectified linear unit. \((u(z)\) for the choice $\sigma(u) = \frac{a u \exp\left[\frac{u^2}{2}\right] + b u \exp\left[\frac{bu^2}{2}\right]}{\exp\left[\frac{u^2}{2}\right] + \exp\left[\frac{bu^2}{2}\right]}\) is left implicit since the inverse is not available in closed form. The same applies for the negative entropy and the Bregman divergence.)

The Lagrangian in (4) expresses a saddle-point problem—a minimization problem on $W$ and a maximization problem on the predictors $\{z_k\}$. We will show that the Lagrangian is concave w.r.t. $\{z_k\}$ leading to a convex dual minimization on $\{\lambda_k\}$. It turns out to be more convenient to work with a single instance Lagrangian rather than (4) which is on the entire training set. This is written as

$$
\mathcal{L}_{\text{MC-LR}}(W, z, \lambda) = (z - y)^T W^T x - e^T \psi(z) + \lambda \left(e^T z - 1 \right).$$

(6)

**Lemma 1.** Eliminating $z$ via maximization in (4) and solving for the Lagrange parameter $\lambda$ via minimization yield the multi-class logistic regression negative log-likelihood in (5).

**Proof.** Since $\psi(z)$ is continuous and differentiable, we differentiate and solve for $z$ in (6). Note that (6) contains a sum of linear and concave (since $\psi(z) = z \log z - z$ is convex) terms on $z$ and is therefore concave. The negative of the Lagrangian is convex and differentiable w.r.t. $z$ and with a linear constraint on $z$, we are guaranteed that the dual is convex (and without any duality gap) [Boyd and Vandenberghe, 2004, Slater, 2014]. We obtain

$$
\log z_k = w_k^T x + \lambda \Rightarrow z_k = \exp\{w_k^T x + \lambda\}.
$$

(7)

(Note that the predictor $z_k$ has a nonlinear dependence on both $W$ and $\lambda$ through the choice of sigmoid: exp.) We eliminate $z$ to obtain the dual w.r.t. $\lambda$ written as

$$
R_{\text{MC-LR}}(W, \lambda) = - \sum_{k=1}^{K} y_k w_k^T x - \lambda + \sum_{k=1}^{K} \exp\{w_k^T x + \lambda\}
$$

$$
= - \sum_{k=1}^{K} y_k w_k^T x - \lambda + \sum_{k=1}^{K} \phi(w_k^T x + \lambda)
$$

$$
= - \sum_{k=1}^{K} y_k \left(w_k^T x + \lambda\right) + \sum_{k=1}^{K} \phi(w_k^T x + \lambda)
$$

(8)

where we have used the fact that $\sum_{k=1}^{K} y_k = 1$. Also $\phi(u) = \exp\{u\}$ is the sigmoid integral corresponding to the choice of sigmoid $\sigma(u) = \exp\{u\}$. Please see section 3.1 and Table 1 for more information on the notation used. It should be understood that we continue to have a minimization problem on $W$ but now augmented with a convex minimization problem on $\lambda$. Differentiating and solving for $\lambda$ in (8), we get
Lagrange parameter \( \lambda \)  

Without the constraints, the predictor attains its maximum for any of the set of Lagrange parameters \( \lambda \). It should be clear from Lemma 1 (that this is a minimization problem, the intuition here is that the maximization problem leads to a predictor to reach \( \lambda \)), which can be combined with the minimization problem on \( z \) and the constraint \( Az = b \) for a single training set pair \( (x, y) \).

\[
-1 + \sum_{k=1}^{K} \exp \{ w_k^T x + \lambda \} = 0 \Rightarrow \lambda = -\log \sum_{k=1}^{K} \exp \{ w_k^T x \}.
\]

Substituting this solution for \( \lambda \) in (8), we get

\[
R_{MC-LR}(W, \lambda(W)) = -\sum_{k=1}^{K} \mathbf{y}_k w_k^T x + \log \sum_{k=1}^{K} \exp \{ w_k^T x \} + \text{constant}
\]

which is identical (up to additive constant terms) to (3).

We can write the dual (with the optimization on \( W \)) as a new MC-LR objective function:

\[
E_{MC-LR}^{(\text{total})}(W, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ -y_n^T W^T x_n - \lambda_n + e^T \phi \left( W^T x_n + \lambda_n e \right) \right] .
\]

It should be clear from Lemma 1 (that this is a minimization problem on \( (W, \{\lambda_n\}) \) despite the presence of the set of Lagrange parameters \( \{\lambda_n\} \). The structure of the objective function strongly indicates that the Lagrange parameter \( \lambda_n \) is almost on the same footing as the set of penultimate layer hidden units \( x_n \): it appears inside the nonlinearity in the form of a new unit with a fixed weight of one and also connects to the loss in the same manner. Noting that \( e^T y_n = 1 \), we rewrite (11) as

\[
E_{MC-LR}^{(\text{total})}(W, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ -y_n^T \left( W^T x_n + \lambda_n e \right) + e^T \phi \left( W^T x_n + \lambda_n e \right) \right]
\]

which is similar to (1) but with the specialization to multi-class classification. This simple observation serves as an underpinning for the entire paper.

### 3.2 Difference of squared \( \ell_2 \) norms Lagrangian

We now embark on clarifying the intuition that led to the Ansatz in (4). Since divergence measures are closely coupled to nonlinearities in neural networks, it can be quite difficult to guess at the right Lagrangian which allows us to move from a saddle-point problem to a dual minimization (on weight matrices and Lagrange parameters). To (initially) remove nonlinearities completely from the picture, consider the following saddle-point Lagrangian with a minimization problem on \( W \), a maximization problem on \( z \) and the constraint \( Az = b \) for a single training set pair \( (x, y) \).

\[
\mathcal{L}_{\ell_2}(W, z, \lambda) = \frac{1}{2} || y - W^T x ||_2^2 - \frac{1}{2} || z - W^T x ||_2^2 + \lambda^T (Az - b).
\]

Without the constraints, the predictor attains its maximum for \( z = W^T x \), the optimal solution and we recover the original unconstrained learning problem on the weights. With the constraints, the maximization problem is not (usually) allowed to reach its unconstrained value with the predictor likewise not allowed to reach \( W^T x \) due to constraint satisfaction. With the constrained maximization problem nested inside the minimization problem, the intuition here is that the maximization problem leads to a predictor \( z \) which depends only on the input \( x \) (and not directly on \( y \)) and satisfies the constraints \( (Az = b) \). Furthermore, elimination of \( z \) leads to a dual minimization problem on \( \lambda \) which can be combined with the minimization problem on \( W \) in exactly the same way as in MC-LR above. After this elimination step, \( W \) is tuned to best fit to the “labels” \( y \) (but with a regularization term obtained from the maximization problem, one that penalizes deviation from the constraints). By this mechanism, the weight gradient of the objective function gets projected into the subspace spanned by the constraints. Consequently, once initial conditions are set up to satisfy the constraints, the network cannot subsequently deviate from them. Since each training set instance \( (x, y) \) is deemed to satisfy \( Ay = b \), we can separately evaluate the gradient term for each training set pair for constraint satisfaction.

**Lemma 2.** If \( Ay = b \), then \( \nabla_W \mathcal{L}_{\ell_2}(W, z(W), \lambda(W)) = 0 \), or in other words the gradient w.r.t. \( W \) of the Lagrangian in (13) with \( z \) and \( \lambda \) set to their optimal values is in the nullspace of \( A \).
where we rewrite it as

\[ z = W^T x + A^T \lambda. \]  

(14)

Substituting this solution for \( z \) in (13), we obtain the dual objective function (while continuing to have a minimization problem on \( W \)):

\[ R_{\ell_2}(W, \lambda) = \frac{1}{2} \| y - W^T x \|_2^2 + \frac{1}{2} A^T AA^T \lambda + \lambda^T AW^T x - \lambda^T b \]

\[ \propto -y^T W^T x - b^T \lambda + \frac{1}{2} x^T WW^T x + x^T WA^T \lambda + \frac{1}{2} A^T AA^T \lambda \]

\[ = -y^T W^T x - b^T \lambda + \frac{1}{2} \| W^T x + A^T \lambda \|_2^2. \]  

(15)

This objective function is similar to the previous one obtained for MC-LR in (8) and to help see the intuition, we rewrite it as

\[ S_{\ell_2}(W, z, \lambda) = -y^T W^T x - y^T A^T \lambda + y^T A^T \lambda - b^T \lambda + \frac{1}{2} \| W^T x + A^T \lambda \|_2^2 \]

\[ = -y^T z + \frac{1}{2} z^T z + A^T (Ay - b) \quad \text{(since } z = W^T x + A^T \lambda) \]

\[ = -y^T z + \frac{1}{2} z^T z \]  

(16)

since \( Ay = b \) and with \( z \) as in (14). This clearly shows the constrained predictor \( z = W^T x + A^T \lambda \) attempting to fit to the labels \( y \).

We now enforce the constraint \( Az = b \) in (14) to get

\[ AW^T x + AA^T \lambda = b \Rightarrow \lambda = \left(AA^T \right)^{-1} \left(b - AW^T x \right) \]  

(17)

provided \( (AA^T)^{-1} \) exists. Using the solution in (17) and eliminating \( \lambda \) from the objective function in (13), we obtain

\[ R_{\ell_2}(W, \lambda(W)) = -y^T W^T x + x^T WQb + \frac{1}{2} x^T WPW^T x \]  

(18)

where \( P \equiv (I - A^T (AA^T)^{-1} A) \) is a projection matrix (with \( P^2 = P \)) and \( Q = A^T (AA^T)^{-1} A \) which can be readily verified. The objective function w.r.t. \( W \) is clearly bounded from below by virtue of the last term in (18). Taking the gradient of \( R_{\ell_2} \) w.r.t. \( W \), we obtain

\[ \nabla_W R_{\ell_2}(W, \lambda(W)) = [-y + Qb + PW^T x] x^T. \]  

(19)

From this, we get

\[ A \nabla_W R_{\ell_2}(W, \lambda(W)) = [-Ay + AQb + APW^T x] x^T = (-Ay + b) x^T = O \]  

(20)

since \( AQ = I, AP = O \) and provided the target \( y \) satisfies \( Ay = b \) which was our starting assumption. \( \square \)

We have shown that the gradient of the effective objective function w.r.t. \( W \) for each training set pair \((x, y)\) obtained by eliminating \( z \) and \( \lambda \) from the Lagrangian in (13) lies in the nullspace of \( A \). This observation may be useful mainly for analysis since actual constraint satisfaction may be computationally more efficient in the dual objective function (written for all training set instances for the sake of completion):
The generalized sigmoid integral is defined as the vector

\[ E^{(\text{total})}_{\ell_2} (W, \{A_n\}) = \sum_{n=1}^{N} \left[ -y_n^T W^T x_n - b_n^T A_n + \frac{1}{2} \| W^T x_n + A^T A_n \|_2^2 \right] \]

\[ = \sum_{n=1}^{N} \left[ -y_n^T (W^T x_n + A^T A_n) + \frac{1}{2} \| W^T x_n + A^T A_n \|_2^2 \right] \text{ (since } Ay_n = b_n) \]

\[ = \sum_{n=1}^{N} \left[ -y_n^T z_n(W, A_n) + \frac{1}{2} \| z_n(W, A_n) \|_2^2 \right] \]

(21)

where the predictor

\[ z_n(W, A_n) \equiv W^T x_n + A^T A_n \]

(22)
as before in (14) but modified to express the dependence on the parameters \( W \) and \( A_n \). The surprising fact that we can augment the penultimate layer units and the final layer weights in this manner has its origin in the difference between the squared \( \ell_2 \) norms used back in (13). Therefore, we have shown that the components of the Lagrange parameter vector \( \lambda \) can be interpreted as additional, penultimate layer hidden units with fixed weights obtained from \( A \). In the remainder of the paper, we generalize this idea to Bregman divergences allowing us to prove the same result for any suitable generalized sigmoid (under the presence of linear equality constraints).

### 3.3 The difference of Bregman divergences Lagrangian

As we move from the specific (MC-LR and \( \ell_2 \)) to the general (Bregman divergence), we define some terms which simplify the notation and development.

**Definition 3.** The generalized sigmoid vector \( \sigma(u) \) is defined as \( \sigma(u) = [\sigma(u_1), \ldots, \sigma(u_K)]^T \) where \( \sigma(u) \) is continuous, differentiable and monotonic \( (\sigma' > 0, \forall u) \).

An example (different from the standard sigmoid) is \( \sigma(u) = \tanh(u) \). Its derivative \( \sigma'(u) = \tanh^2(u) > 0, \forall u \in (-\infty, \infty) \).

**Definition 4.** The generalized sigmoid integral is defined as the vector \( \phi(u) = [\phi(u_1), \ldots, \phi(u_K)]^T \) where \( \phi(u) = \int_{-\infty}^{u} \sigma(v) dv \).

Continuing the \( \sigma(u) = \tanh(u) \) example, the sigmoid integral for \( \sigma(u) = \tanh(u) \) is \( \phi(u) = \log \cosh(u) \).

**Definition 5.** The generalized inverse sigmoid is defined as a vector \( u(z) = [u(z_1), \ldots, u(z_K)]^T \) where \( u(z) = \sigma^{-1}(z) = (\phi')^{-1}(z) \).

The inverse sigmoid for \( \sigma(u) = \tanh(u) \) is \( u(z) = \frac{1}{2} \log \frac{1+z}{1-z} \).

**Definition 6.** The generalized negative entropy \( \psi(z) \) is defined as \( z^T u(z) - e^T \phi(u(z)) \).

For \( \sigma(u) = \tanh(u) \), the negative entropy \( \psi(z) = \frac{1}{2} \left[ (1+z) \log(1+z) + (1-z) \log(1-z) \right] \) and \( \phi(u(z)) = \frac{1}{2} \log(1 - z^2) \). The generalized negative entropy \( \psi(z) \) is related to the Legendre transform of \( \phi(u) \) (and can be derived from Legendre-Fenchel duality theory [Fenchel, 2014] and Mjolsness and Garrett, 1990) but this relationship is not emphasized in the paper.

**Corollary 7.** The generalized negative entropy \( \psi(z) \) is convex.

**Proof.** Since \( \psi(z) \) is a sum of individual functions \( \psi(z) \), we just need to show that \( \psi(z) \) is convex. The derivative of \( \psi(z) \) is

\[ \psi'(z) = u(z) + zu'(z) - \phi'(u(z))u'(z) = u(z) + zu'(z) - zu'(z) = u(z) \]

(23)
since \( u(z) = (\phi')^{-1}(z) \). The second derivative \( \psi''(z) \) is
ψ''(z) = u'(z) = \frac{1}{\sigma'(u(z))} > 0 \quad (24)

since \( u(z) = \sigma^{-1}(z) \) and \( \sigma'(u) > 0 \). Therefore the generalized negative entropy is convex.

We can directly show the convexity of the negative entropy \( \psi(z) \) for \( \sigma(u) = \tanh(u) \) by evaluating \( \psi''(z) = u'(z) = \frac{d}{dz} \left( \frac{1}{2} \log \frac{1+z}{1-z} \right) = \frac{1}{1-z^2}, \forall z \in [-1,1] \). We now set up the Bregman divergence [Bregman, 1967] for the convex negative entropy function \( \psi(z) \).

**Definition 8.** The Bregman divergence for a convex, differentiable function \( \psi(z) \) is defined as

\[
B(z||v) = \psi(z) - \psi(v) - \psi'(v)(z - v) \quad (25)
\]

This can be extended to the generalized negative entropy \( \psi(z) \) but the notation becomes a bit more complex. For the sake of completeness, the Bregman divergence for \( \psi(z) \) is written as

\[
B(z||v) = \mathbf{e}^T (\psi(z) - \psi(v)) - (\nabla \psi(v))^T (z - v) \quad (26)
\]

where \( \nabla \psi(v) \) is the gradient vector of the generalized negative entropy defined as \( \nabla \psi(v) \equiv [\psi'(v_1), \ldots, \psi'(v_K)]^T \).

This definition can be used to build the Bregman divergence for the generalized negative entropy \( \psi(z) \) written as

\[
B(z||v) = \psi(z) - \psi(v) - \psi'(v)(z - v) \\
= u(z) - \phi(u(z)) - vu(v) + \phi(u(v)) - u(v)(z - v) \\
= z [u(z) - u(v)] - \phi(u(z)) + \phi(u(v)). \quad (27)
\]

Therefore, the Bregman divergence for the choice of \( \sigma(u) = \tanh(u) \) is

\[
B_{\tanh}(z||v) = z \left[ \frac{1}{2} \log \frac{1+z}{1-z} - \frac{1}{2} \log \frac{1+v}{1-v} \right] - \frac{1}{2} \log (1 - z^2) + \frac{1}{2} \log (1 - v^2) \]

\[
= \frac{1}{2} \left( (1+z) \log \frac{1+z}{1+v} + (1-z) \log \frac{1-z}{1-v} \right) \quad (28)
\]

which is the Kullback-Leibler (KL) divergence for a binary random variable \( Z \) taking values in \( \{-1,1\} \) which is what we would expect once we make the identification that \( z = 2 \Pr(Z = 1) - 1 \) with a similar identification for \( v \).

**Corollary 9.** The Bregman divergence \( B_{\text{gen} \psi}(z||v) \) is convex in \( z \) for the choice of the generalized negative entropy function \( \psi(z) \).

**Proof.** Since \( B_{\text{gen} \psi}(z||v) \) is a summation of \( \psi(z) \) and a term linear in \( z \), it is convex in \( z \) due to the convexity of \( \psi(z) \) (shown earlier in Lemma 7). 

We now describe the crux of one of the basic ideas in this paper: that the difference between squared \( \ell_2 \) norms in [13] when generalized to the difference of Bregman divergences leads to a dual minimization problem wherein the Lagrange parameters are additional penultimate layer hidden units. In [13] we showed that nesting a maximization problem on the constrained predictor \( z \) inside the overall minimization problem w.r.t. \( W \) had two consequences: (i) eliminating \( z \) led to a minimization problem on \( \lambda \); (ii) the saddle-point problem led to opposing forces—from the target \( y \) and from the input \( x \)—which led to projected gradients which satisfied the constraints. Furthermore, the Lagrange parameters carried the interpretation of penultimate layer hidden units (albeit in a final layer with a linear output unit) via the form of the dual minimization problem in [21]. We now generalize the difference of squared \( \ell_2 \) norms to the difference of Bregman divergences and show that the same interpretation holds for suitable nonlinearities in the output layer.
From the generalized negative entropy Bregman divergence, we form the difference of Bregman divergences to get

\[
B_{\text{gensig}}(y||v) - B_{\text{gensig}}(z||v) = (z - y)u(v) + yu(y) - \phi(u(y)) - zu(z) + \phi(u(z)).
\]

(29)

**Lemma 10.** The difference of Bregman divergences is linear in the weight matrix \(W\) for the choice of the convex generalized negative entropy vector \(\psi(z)\) and for \(v = \sigma(W^T x)\).

**Proof.** This is a straightforward consequence of the two choices.

\[
B_{\text{gensig}}(y||v) - B_{\text{gensig}}(z||v) = y(u(y) - u(v)) - \phi(u(y)) + \phi(u(v)) - [z(u(z) - u(v)) - \phi(u(z)) + \phi(u(v))]
\]

\[
= (z - y)u(v) + yu(y) - \phi(u(y)) - zu(z) + \phi(u(z))
\]

\[
= (z - y)u(v) - zu(z) + \phi(u(z)) + \text{terms independent of } z
\]

\[
= (z - y)u(v) - \psi(z) + \text{terms independent of } z.
\]

(30)

We write this for a single instance as

\[
B_{\text{gensig}}(y||v) - B_{\text{gensig}}(z||v) \propto (z - y)^T u(v) - z^T u(z) + e^T \psi(u(z)).
\]

(31)

\[
= (z - y)^T u(v) - e^T \psi(z).
\]

(32)

Note that the difference of Bregman divergences depends on \(v\) only through \(u(v)\). We now set \(v = \sigma(W^T x)\) and rewrite the difference between Bregman divergences using terms that only depend on \(W, x\) and \(z\) to get

\[
B_{\text{gensig}}(y||\sigma(W^T x)) - B_{\text{gensig}}(z||\sigma(W^T x)) \propto (z - y)^T W^T x - e^T \psi(z)
\]

(33)

which is linear in the weight matrix \(W\).

**Corollary 11.** The difference of Bregman divergences for the choice of \(\phi(z) = \frac{z^2}{2}\) is identical to the difference of squared \(\ell_2\) norms in (13).

**Proof.** We evaluate the difference of Bregman divergences for \(\phi(z) = \frac{z^2}{2}\) by substituting this choice of \(\phi(z)\) in (29) to get

\[
B_{\ell_2}(y||v) - B_{\ell_2}(z||v) = (z - y)v + y^2 - \frac{y^2}{2} - z^2 + \frac{z^2}{2}
\]

\[
= \frac{1}{2}(y - v)^2 - \frac{1}{2}(z - v)^2
\]

(34)

which when extended to the entire set of hidden units is the difference between the squared \(\ell_2\) norms as in (13).

The general saddle-point problem can now be expressed (for a single training set pair) as

\[
\min_w \max_z B_{\text{gensig}}(y||\sigma(W^T x)) - B_{\text{gensig}}(z||\sigma(W^T x)) \propto \min_w \max_z (z - y)^T W^T x - e^T \psi(z)
\]

(35)

subject to \(A z = b\).

The order of the maximization and minimization matters. It is precisely because we have introduced a maximization problem on \(z\) inside a minimization problem on the weights \(W\) that we are able to obtain a dual minimization problem on the Lagrange parameters in exactly the same manner as in multi-class logistic regression. This will have significant implications later. The difference of Bregman divergences is concave in \(z\). Note that the weight matrix \(W\) appears linearly in (33) due to the choice of \(v = \sigma(W^T x)\) which produces
the correct generalization of (6). We add the linear constraints $Az = b$ as before and write the Lagrangian for a single instance

$$L_{\text{gensig}}(W, z, \lambda) = (z - y)^T W^T x - e^T \psi(z) + \lambda^T (Az - b)$$

which can be expanded to the entire training set as

$$L_{\text{gensig}}^{\text{(total)}}(W, \{z_n\}, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ (z_n - y_n)^T W^T x_n - e^T \psi(z_n) + \lambda_n^T (Az_n - b_n) \right].$$

where the negative entropy $\psi(z) = z^T u(z) - e^T \phi(u(z))$. The final saddle-point Lagrangian contains a minimization problem on $W$ and a maximization problem on $\{z_n\}$ with the unknown Lagrange parameter vectors $\{\lambda_n\}$ handling the linear constraints. Note that $\phi(u(z))$ lurking inside $\psi(z)$ is a generalized sigmoid integral (as per Definition 4) with $u(z)$ being the matched generalized inverse sigmoid. The generalized sigmoid integral is not restricted to the exponential function.

We now show that the generalized dual objective function on $\{\lambda_n\}$ (along with a minimization problem on $W$) is of the same form as the MC-LR dual objective function (11) and is written as

$$E_{\text{gensig}}^{\text{(total)}}(W, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ -y_n^T (W^T x_n + A^T \lambda_n) + e^T \phi(W^T x_n + A^T \lambda_n) \right].$$

**Lemma 12.** Eliminating $z$ via maximization in (37) and solving for the Lagrange parameter vector $\lambda$ via maximization yield the dual objective function in (38) provided $u(z)$ is set to $\phi^{-1}(z)$.

**Proof.** Since $\psi(z)$ is continuous and differentiable, we differentiate and solve for $z$ in (37). This is simpler to write for the single instance Lagrangian in (36). Differentiating w.r.t. $z$ and setting the result to 0, we get

$$W^T x - u(z) - z \odot \nabla u(z) + \nabla \phi(u(z)) \odot \nabla u(z) + A^T \lambda = 0.$$  

(Please see section 3.1 on the notation used for an explanation of these terms.) Since $\phi'(u(z)) = \phi'((\phi')^{-1}(z)) = z$, we have $z = \nabla u \phi(u(z))$. From this we get

$$u(z) = W^T x + A^T \lambda$$

and therefore

$$z^T W^T x - z^T u(z) + z^T A^T \lambda = 0.$$  

(41)

Substituting this in (37), we get the dual objective function (along with a minimization problem on $W$) written for just a single training set instance to be

$$E_{\text{gensig}}(W, \lambda) = \left[ -y^T W^T x - b^T \lambda + e^T \phi(W^T x + A^T \lambda) \right]$$

$$= \left[ -y^T (W^T x + A^T \lambda) + e^T \phi(W^T x + A^T \lambda) \right]$$

(since $Ay = b$)

$$= \left[ -y^T u + e^T \phi(u) \right]$$

(42)

where $u \equiv W^T x + A^T \lambda$ is the linear predictor (with $z = \sigma(u)$ being the nonlinear predictor). Equation (42) when expanded to the entire training set yields (38) and can be rewritten in component-wise form as

$$E_{\text{gensig}}^{\text{(total)}}(W, \{\lambda_n\}) = \sum_{n=1}^{N} \left[ -y_{nk} \left( \sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i=1}^{I} a_{ik} \lambda_{ni} \right) + \sum_{k=1}^{K} \phi \left( \sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i=1}^{I} a_{ik} \lambda_{ni} \right) \right]$$

$$= \sum_{n=1}^{N} \left[ -y_{nk} u_{nk} + \sum_{k=1}^{K} \phi (u_{nk}) \right]$$

(43)
where
\[ u_{nk} = \sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i=1}^{I} a_{ik} \lambda_{ni}, \quad (44) \]

the component-wise linear predictor counterpart to \( u = W^T x + A^T \lambda \). We have shown that we get a minimization problem on both the weights and the Lagrange parameter vectors (one per training set instance) in a similar manner to the case of multi-class logistic regression. We stress that \( z = \sigma(u) \) requires \( \sigma(u) = \phi'(u) : \) the chosen nonlinearity and the choice of \( \phi(u) \) in the loss function in (42) are in lockstep. This is a departure from standard practice in present day deployments of feedforward neural networks.

The minimization problem in (38) is valid for any generalized sigmoid \( \sigma(u) \) provided it is continuous, differentiable and monotonic. We state without proof that the dual objective function is convex w.r.t. both the top layer weights \( W \) and the Lagrange parameter vectors \( \lambda \). However, since we plan to deploy standard stochastic gradient descent methods for optimization, this fact is not leveraged here.

We end by showing that the predictor \( z \) satisfies the linear equality constraints.

**Corollary 13.** The nonlinear predictor \( z = \sigma(u) = \sigma(W^T x + A^T \lambda) \) satisfies the constraints \( Az = b \) for the optimal setting of the Lagrange parameter vector \( \lambda \).

**Proof.** We differentiate (38) w.r.t. \( \lambda_n \) and set the result to 0 to obtain
\[ \sum_{k=1}^{K} a_{ik} \phi'(\sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i'=1}^{I} a_{i'k} \lambda_{ni'}) = b_{ni}, \forall i \in \{1, \ldots, I\} \quad (45) \]
or
\[ Az_n = b_n, \forall n \quad (46) \]
at the optimal value of the Lagrange parameter vector \( \lambda_n \) and
\[ z_{nk} = \phi'(\sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i=1}^{I} a_{ik} \lambda_{ni}) = \sigma\left(\sum_{j=1}^{J} w_{jk} x_{nj} + \sum_{i=1}^{I} a_{ik} \lambda_{ni}\right), \forall n, k, \quad (47) \]
and we are done. \( \square \)

## 4 Applications

### 4.1 Synthetic Equality Constraints

We now demonstrate the incorporation of equality constraints through a simple example. To this end, we construct a feedforward network for the XOR problem using 4 fully connected layers. The last layer (fc4) is a linear classifier with a single output whereas the previous layer (fc3) converts the fc2 outputs into new features which are easier to classify than the original coordinates. Consequently, we visualize the fc3 weights as enacting linear constraints on the fc2 outputs in the form \( Ax_2 = b \) where \( A \) is the set of weights corresponding to the fc3 layer with \( x_2 \) being the output of the fc2 layer and \( b \) being the set of final XOR features. We train this network in PyTorch using a standard approach with 2000 training set samples in \( \mathbb{R}^2 \).

The network architecture is as follows: 10 weights in fc1 (2 units to 5 units), 50 weights in fc2 (5 units to 10 units), 40 weights in fc3 (10 units to 4 units) and 4 weights in fc4 (4 units to 1 unit). Each set of weights in each layer is accompanied by bias weights as well. After training, we extract the weights corresponding to \( A \) (the weights of the fc3 layer) and store them.

Next, we set up our constraint satisfaction network. The goal of this network is to begin with fresh inputs in \( \mathbb{R}^2 \) and map them to the outputs of the previous network’s fc2 layer \( x_2 \) which are the new targets \( y \) while satisfying the constraints \( (Ax_2 = b) \). This is explained in greater detail. Assume we have new inputs \( x_0^{(\text{new})} \). These are sent into the XOR network to produce the output of the fc2 layer \( x_2 \) which we now call \( y \), the new targets. But, we also know that the targets \( y \) satisfy additional constraints in the form of the
XOR network’s fc3 layer. Therefore, if we construct a new network with \( y \) being the target of the fc2 layer then the new network (henceforth XOR Lagrange) has constraints \( A \hat{x}^{(new)}_2 = Ay = Ax_2 \) which need to be enforced. Since the XOR fc3 layer maps 10 units to 4 units, there are 4 constraints for each \( x^{(new)}_2 \) in XOR Lagrange. To enforce these, we set up a custom layer which has additional fixed weights (mapping 10 units to 4 units) in the form of \( A \) and a set of Lagrange parameters (4 per training or test pattern) which need to be obtained. We train the new XOR Lagrange network in the same way as the XOR network but with one crucial difference. In each epoch and for each batch, we use a constraint satisfaction network to solve for the 4 Lagrange parameters for each pattern in each batch. A standard gradient descent approach with a step size solver is used. We use a threshold of \( 5 \times 10^{-3} \) for the average change in the loss function w.r.t. \( A \) (the Lagrange parameters)—essentially a standard BCE loss—and a threshold of \( 1.0 \times 10^{-6} \) for the step-size parameter (where the search begins with \( \alpha \) the step-size parameter set to 0.1 and then halved each time if too high). If convergence is not achieved, we stop after 100 iterations of constraint satisfaction. Note that we do not need to completely solve for constraint satisfaction in each epoch but have chosen to do so in this first work.

XOR Lagrange was executed 1000 times on a fresh input (with 2000 patterns) with the results shown in Figure 1. We discovered a very common pattern in the optimization. Initially for every fresh input \( x^{(new)}_0, x^{(new)}_2 \) is far away from \( y \) and the constraint satisfaction solver can take many iterations to obtain \( A \hat{x}^{(new)}_2 \approx Ay \) (and note that both \( x^{(new)}_2 \) and \( y \) are the outputs of sigmoids). Then, as optimization proceeds, the number of constraint satisfaction iterations steadily decreases until \( x^{(new)}_2 \approx y \) (and we always execute for 100 epochs). In the figure, we depict this progression for the maximum, minimum and mean number of iterations. The loss function in each epoch is also shown (in lockstep) for the sake of comparison. While the mean number of constraint satisfaction iterations trends lower, we do see instances of large numbers of iterations in the maximum case. This suggests that we need to explore more sophisticated optimization schemes in the future.

We conclude with an initial foray into improved constraint satisfaction. In the above set of experiments, we did not propagate the Lagrange parameters across epochs. This causes the constraint satisfaction subsystem to repeatedly solve for the Lagrange parameters from scratch which is wasteful since we have a global optimization problem on both \( W \) and \( \{\lambda_n\} \). To amend this, we treat \( \{\lambda_n\} \) as state variables and initialize the constraint satisfaction search in each epoch using the results from the previous one. The only parameter value change from the above is a threshold of \( 1 \times 10^{-3} \) for the average change in the loss function w.r.t. the Lagrange parameters with this lower value chosen due to the improved constraint satisfaction subsystem. Despite this tighter threshold, the total number of iterations for constraint satisfaction is lowered as can be seen in Figure 2. The figure also depicts the evolution towards convergence of a suitable Lagrange parameter norm \( ||A|| \).

5 Discussion

The motivation behind the work is to endow neural networks with constraint satisfaction capabilities. We have shown this can be accomplished by appealing to a saddle-point principle—the difference of Bregman divergences—with constraints added to a maximization problem which is carefully defined on a new set of auxiliary predictor variables. When these predictors are eliminated from the Lagrangian, we obtain a dual minimization problem on the Lagrange parameters (one per training set instance). The price of admission for constraint satisfaction therefore is an expansion of the penultimate hidden layer with additional Lagrange parameter units (and fixed weights corresponding to the constraints). Solutions for the Lagrange parameters are required in addition to weight learning with further optimization needed during testing. The advantage of this formulation is that we have a single minimization problem (as opposed to a saddle-point problem) with the unusual interpretation of Lagrange parameters as hidden units. Immediate future work will contend not only with linear inequality constraints (perhaps achieved via non-negativity constraints on the Lagrange parameters) but nonlinear equality constraints which may require modifications of the basic framework. We envisage a host of applications stemming from this work, driven by domain scientists who can now attempt to impose more structure during learning using application-specific constraints.
Figure 1: **XOR Lagrange.** In each subplot, we show training progress with constraint satisfaction. In each top subplot, the constraint satisfaction progress is depicted with its loss counterpart proceeding in lockstep below. The maximum, minimum and mean iterations (for 1000 runs) are shown in the left, middle and right subplots respectively.
Figure 2: **XOR Lagrange with history**: In each top subplot, the constraint satisfaction progress is depicted with its loss counterpart proceeding in lockstep immediately below. The bottom set of plots show the evolution of the Lagrange parameters via their norm $||\lambda||$. The maximum, minimum and mean iterations (for 1000 runs) are shown in the left, middle and right subplots respectively.
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