Equilibria of Iterative Softmax and Critical Temperatures for Intermittent Search in Self-Organizing Neural Networks

Peter Tiňo
School of Computer Science
The University of Birmingham
Birmingham B15 2TT, UK

Abstract

Kwok and Smith (2005) recently proposed a new kind of optimization dynamics using self-organizing neural networks (SONN) driven by softmax weight renormalization. Such dynamics is capable of powerful intermittent search for high-quality solutions in difficult assignment optimization problems. However, the search is sensitive to temperature setting in the softmax renormalization step. It has been hypothesized that the optimal temperature setting corresponds to the symmetry breaking bifurcation of equilibria of the renormalization step, when viewed as an autonomous dynamical system called iterative softmax (ISM). We rigorously analyze equilibria of ISM by determining their number, position and stability types. It is shown that most fixed points exist in the neighborhood of the maximum entropy equilibrium $\overline{\mathbf{w}} = (N^{-1}, N^{-1}, ..., N^{-1})$, where N is the ISM dimensionality. We calculate the exact rate of decrease in the number of ISM equilibria as one moves away from $\overline{\mathbf{w}}$. Bounds on temperatures guaranteeing different stability types of ISM equilibria are also derived. Moreover, we offer *analytical* approximations to the critical symmetry breaking bifurcation temperatures that are in good agreement with those found by numerical investigations. So far the critical temperatures have been determined only via trial-and-error numerical simulations. On a set of N-queens problems for a wide range of problem sizes N, the analytically determined critical temperatures predict the optimal working temperatures for SONN intermittent search very well. It is also shown that no intermittent search can exist in SONN for temperatures greater than 1/2.

1 Introduction

Since the pioneering work of Hopfield (1982), adaptation of neural computation techniques to solving difficult combinatorial optimization problems has proved useful in numerous application domains (Smith, 1999). In particular, a self-organizing neural network (SONN) was proposed as a general methodology for solving 0-1 assignment problems in (Smith, 1995). The methodology has been successfully applied in a wide variety of applications, from assembly line sequencing to frequency assignment in mobile communications (see e.g. (Smith, Palaniswami, and Krishnamoorthy, 1998)).

The key difference between the traditional self-organizing maps (SOM) (Kohonen, 1982) and SONN lies in the notion of neighborhood of the winning unit (the unit most responsive to the current input). In the Kohonen-type SOM, neural units play the role of codebook vectors in a constrained vector quantization of the input space. Close units on the map represent close regions of the input space. As the map develops, the notion of "closeness" on the map changes only in scale, while the topology of neighborhood relations remains unchanged. In contrast, SONN adopt a more flexible notion of the winning unit neighborhood. Neural units represent partial solutions to an assignment optimization problem. The criterion for closeness of two units is their relative performance in solving the optimization task. In this view, neighborhood of the winning unit contains only relatively successful partial assignment solutions to the optimization task being solved. There is no pre-determined neighborhood topology on the neural units. However, both SOM and SONN share the philosophy of neighborhood-based updating of the parameters (weights). The winner unit, as well as units from its neighborhood are modified to better respond to the current input stimulus.

Searching for 0-1 solutions in general assignment optimization problems can be made more effective when performed in a continuous domain, with values in the interval $(0, 1)$ representing partial (soft) assignments (e.g. (Kosowsky and Yuille, 1994)). Typically the softmax function is employed to ensure that elements within a set of positive parameters sum up to one. The softmax function was incorporated into SONN in (Guerrero et al., 2002) and was used in other optimization frameworks e.g. in (Gold and Rangarajan, 1996; Rangarajan, 2000). When endowed with a physics-based Boltzmann distribution interpretation, the softmax function contains a free parameter - temperature T (or inverse temperature T^{-1}). As the system cools down, the assignments become increasingly crisp.

Recently, interesting observations have been made regarding the appropriate values of the temperature parameter when solving assignment problems with SONN endowed with softmax renormalization of the weight parameters (Kwok and Smith, 2002, 2004). There is a critical temperature T_* at which the SONN achieves superior performance in terms of both quality and efficiency. It has been suggested that the critical temperature may be closely related to the symmetry breaking bifurcation of equilibria in the autonomous softmax dynamics (Kwok and Smith, 2003). Even of greater interest is the finding that at T_*, when the neighborhood size and learning rate are kept fixed at appropriate values, SONN is capable of powerful intermittent search through a multitude of high quality solutions represented as meta-stable states of the SONN dynamics (Kwok and Smith, 2005). Kwok and Smith (2005) numerically studied global dynamical properties of SONN in the intermittent search mode and argued that such models display characteristics of systems at the edge-of chaos (Langton, 1990; Crutchfield and Young, 1990).

In this contribution we attempt to shed more light on the phenomenon of critical temperatures and intermittent search in SONN. In particular, since the critical temperature is closely related to bifurcations of equilibria in autonomous iterative softmax systems (ISM), we rigorously analyze the number, position and stability types of fixed points of ISM. Moreover, we offer analytical approximations to the critical temperature, as a function of the ISM dimensionality. So far the critical temperatures have been determined only via trial-and-error numerical investigations.

The paper has the following organization: After a brief introduction to SONN in section 2, we formally define ISM in section 3. The numbers and positions of ISM equilibria are studied in section 4, while their stability is investigated in section 5. Analytical approximations to the critical temperature for SONN intermittent search are derived and verified in section 6. The paper is concluded by summarizing key findings in section 7.

2 Self-Organizing Neural Network with softmax weight renormalization

In this section we briefly introduce Self-Organizing Neural Network (SONN) endowed with weight renormalization for solving assignment optimization problems (see e.g. (Kwok and Smith, 2005)). Consider a finite set of "inputs" $j \in \mathcal{J} = \{1, 2, ..., M\}$ that need to be assigned to "outputs" $i \in \mathcal{I} = \{1, 2, ..., N\}$, so that a global cost (potential) $Q(\mathcal{A})$ of an assignment $\mathcal{A} : \mathcal{J} \to \mathcal{I}$ is minimized. Partial cost of assigning $j \in \mathcal{J}$ to $i \in \mathcal{I}$ is denoted by $V(i, j)$. Both the input and output elements $j \in \mathcal{J}$ and $i \in \mathcal{I}$, respectively, are represented through one-hot-encoding, i.e. there is one input and one output unit exclusively devoted to each input and output element, respectively. The "strength" of assigning j to i is represented by the "weight" $w_{i,j} \in [0, 1]$.

The SONN algorithm consists of the following steps:

1. Initialize connection weights $w_{i,j}$, $j \in \mathcal{J}$, $i \in \mathcal{I}$, to random values around 0.5.

2. Choose at random an input item $j_c \in \mathcal{J}$ and calculate partial costs $V(i, j_c)$, $i \in \mathcal{I}$, of all possible assignments of j_c.

3. The winner output node $i(j_c) \in \mathcal{I}$ is the one that minimizes $V(i, j_c)$, i.e. $i(j_c) = \mathrm{argmin}_{i \in \mathcal{I}} V(i, j_c)$.

   The neighborhood $\mathcal{B}_L(i(j_c))$ of size L of the winner node $i(j_c)$ consist of L nodes $i \neq i(j_c)$ that yield the smallest partial costs $V(i, j_c)$.

4. Weights of nodes $i \in \mathcal{B}_L(i(j_c))$ get strengthened, those outside $\mathcal{B}_L(i(j_c))$ are left unchanged:

$$w_{i,j_c} \leftarrow w_{i,j_c} + \eta(i)(1 - w_{i,j_c}), \quad i \in \mathcal{B}_L(i(j_c)),$$

   where

$$\eta(i) = \beta \exp\left\{ -\frac{|V(i(j_c), j_c) - V(i, j_c)|}{|V(k(j_c), j_c) - V(i, j_c)|} \right\},$$

   and $k(j_c) = \mathrm{argmax}_{i \in \mathcal{I}} V(i, j_c)$.

5. Weights[1] $\mathbf{w}_j = (w_{1,j}, w_{2,j}, ..., w_{N,j})'$ for each input node $j \in \mathcal{J}$ are normalized using softmax

$$w_{i,j} \leftarrow \frac{\exp(\frac{w_{i,j}}{T})}{\sum_{k=1}^{N} \exp(\frac{w_{k,j}}{T})}.$$

6. Repeat from step 2 until all inputs $j_c \in \mathcal{J}$ have been selected (one epoch).

[1]here $'$ denotes the transpose operator

Even though the soft assignments $w_{i,j}$ evolve in continuous space, when needed, a 0-1 assignment solution can be produced by imposing $\mathcal{A}(j) = i$ if and only if $i = \text{argmax}_{k \in \mathcal{I}} w_{k,j}$.

A frequently studied (NP-hard) assignment optimization problem in case of SONN is the N-queen problem (e.g. (Kwok and Smith, 2004, 2005)): place N queens onto an $N \times N$ chessboard without attacking each other. In this case $\mathcal{J} = \{1, 2, ..., N\}$ and $\mathcal{I} = \{1, 2, ..., N\}$ index the columns and rows, respectively, of the chessboard. Partial cost $V(i, j)$ evaluates the diagonal and column contributions[2] to the global cost Q of placing a queen on column j of row i. For more details, see (Kwok and Smith, 2004, 2005).

Many neural-based approaches and heuristic techniques have been proposed to solve the N-queen problem (e.g. (Minton et al., 1992; Tagliarini and Page, 1987)). Previous SONN studies of the N-queen problem used the problem as a convenient testbed for illustrating optimization capabilities of SONN, without intending to devise the most efficient algorithm. The N-queen problem is used in this study in a similar manner.

Kwok and Smith (2003, 2005) argue that step 5 of the SONN algorithm is crucial for intermittent search by SONN for globally optimal assignment solutions. In particular, they note that temperatures at which symmetry breaking bifurcation of equilibria of the renormalization procedure in step 5 occur correspond to temperatures at which optimal (both in terms of quality and quantity of found solutions) intermittent search takes place. In the following sections we rigorously analyze equilibria of softmax viewed as an autonomous dynamical system. Our findings will later allow us to formulate *analytical* approximations to the critical temperatures at which symmetry breaking bifurcations of the softmax renormalization dynamics take place.

3 Iterative softmax

Denote the $(N-1)$-dimensional simplex in $\mathbb{R}^N$ by S_{N-1}, i.e.

$$S_{N-1} = \{\mathbf{w} = (w_1, w_2, ..., w_N)' \in \mathbb{R}^N \mid w_i \geq 0, i = 1, 2, ..., N, \text{ and } \sum_{i=1}^{N} w_i = 1\}. \quad (1)$$

Interior of S_{N-1} is denoted by S^0_{N-1}:

$$S^0_{N-1} = \{\mathbf{w} \in \mathbb{R}^N \mid w_i > 0, i = 1, 2, ..., N, \text{ and } \sum_{i=1}^{N} w_i = 1\}. \quad (2)$$

Given a parameter $T > 0$ (the "temperature"), the softmax maps $\mathbb{R}^N$ into S^0_{N-1}:

$$\mathbf{w} \mapsto \mathbf{F}(\mathbf{w}; T) = (F_1(\mathbf{w}; T), F_2(\mathbf{w}; T), ..., F_N(\mathbf{w}; T))', \quad (3)$$

where

$$F_i(\mathbf{w}; T) = \frac{\exp(\frac{w_i}{T})}{\sum_{k=1}^{N} \exp(\frac{w_k}{T})}, \quad i = 1, 2, ..., N. \quad (4)$$

[2]in the sense of directions on the chessboard

We will denote the common normalization factor of F_i's by $Z(\mathbf{w};T)$, i.e.

$$Z(\mathbf{w};T) = \sum_{k=1}^{N} \exp(\frac{w_k}{T}). \tag{5}$$

Linearization of $\mathbf{F}$ around $\mathbf{w} \in S^0_{N-1}$ is given by the Jacobian $J(\mathbf{w};T)$, the (i,j)-th element of which reads

$$J(\mathbf{w};T)_{i,j} = \frac{1}{T}[\delta_{i,j}F_i(\mathbf{w};T) - F_i(\mathbf{w};T)F_j(\mathbf{w};T)], \tag{6}$$

where $\delta_{i,j} = 1$ iff $i = j$ and $\delta_{i,j} = 0$ otherwise. The Jacobian is a symmetric $N \times N$ matrix.

The softmax map $\mathbf{F}$ induces on S^0_{N-1} a discrete time dynamics

$$\mathbf{w}(t+1) = \mathbf{F}(\mathbf{w}(t);T), \tag{7}$$

sometimes referred to as *Iterative Softmax* (ISM). In the next section we study the relationship between the number and position of equilibria of ISM and the temperature parameter T. We study systems for $N \geq 2$.

4 Fixed points of Iterative Softmax

Recall that $\mathbf{w} \in S^0_{N-1}$ is a fixed point (equilibrium) of the ISM dynamics driven by $\mathbf{F}$, if $\mathbf{w} = \mathbf{F}(\mathbf{w})$. It is easy to see that for any temperature setting[3] there is always at least one fixed point of ISM (7).

Lemma 4.1 *The maximum entropy point* $\overline{\mathbf{w}} = (N^{-1}, N^{-1}, ..., N^{-1})' \in S^0_{N-1}$ *is a fixed point of ISM (7) for any* $T \in \mathbb{R}$.

Proof: The result directly follows from $\bar{w}_1 = \bar{w}_2 = ... = \bar{w}_N$. *Q.E.D.*

There is a strong structure in the fixed points of ISM - coordinates of any fixed point of ISM can take on only up to two distinct values.

Theorem 4.2 *Except for the maximum entropy fixed point* $\overline{\mathbf{w}} = (N^{-1}, ..., N^{-1})'$, *for all the other fixed points* $\mathbf{w} = (w_1, w_2, ..., w_N)'$ *of ISM (7) it holds:* $w_i \in \{\gamma_1(\mathbf{w};T), \gamma_2(\mathbf{w};T)\}$, $i = 1, 2, ..., N$, *where* $\gamma_1(\mathbf{w};T) > N^{-1}$ *and* $\gamma_2(\mathbf{w};T) < N^{-1}$ *are the two solutions of* $Z(\mathbf{w};T) \cdot x = \exp(\frac{x}{T})$.

Proof: We have

$$w_i = F_i(\mathbf{w};T) = \frac{\exp(\frac{w_i}{T})}{Z(\mathbf{w};T)}, \quad i = 1, 2, ..., N.$$

[3]In ISM, T is usually positive, but this claim is true for any $T \in \mathbb{R}$.

That means

$$Z(\mathbf{w};T)\cdot w_i = \exp(\frac{w_i}{T}),$$

and so all the coordinates of $\mathbf{w}$ must lie on the intersection of the line $Z(\mathbf{w};T)\cdot x$ and the exponential function $\exp(\frac{x}{T})$. Since the exponential is a convex function, any line can intersect with it in at most two points.

Because $\mathbf{w} \neq \overline{\mathbf{w}}$, there must be a coordinate w_i of $\mathbf{w}$, such that $w_i \neq N^{-1}$.

If $w_i < N^{-1}$, then (since $\mathbf{w} \in S^0_{N-1}$) there exists another coordinate w_j of $\mathbf{w}$, such that $w_j > N^{-1}$. By the argument above, all the other coordinates of $\mathbf{w}$ must be equal to either w_i or w_j. In addition, w_i, w_j are solutions of $Z(\mathbf{w};T)\cdot x = \exp(\frac{x}{T})$.

The case $w_i > N^{-1}$ can be treated analogously. *Q.E.D.*

We will often write the larger of the two fixed-point coordinates as

$$\gamma_1(\mathbf{w};T) = \alpha N^{-1}, \quad \alpha \in (1,N). \tag{8}$$

Theorem 4.3 *Fix $\alpha \in (1,N)$ and write $\gamma_1 = \alpha N^{-1}$. Let ℓ_{min} be the smallest natural number greater than $(\alpha-1)/\gamma_1$. Then, for $\ell \in \{\ell_{min}, \ell_{min}+1, ..., N-1\}$, at temperature*

$$T_e(\gamma_1; N, \ell) = (\alpha - 1)\left[-\ell \cdot \ln\left(1 - \frac{\alpha-1}{\ell\gamma_1}\right)\right]^{-1}, \tag{9}$$

there exist $\binom{N}{\ell}$ distinct fixed points of ISM (7), with $(N-\ell)$ coordinates having value γ_1 and ℓ coordinates equal to

$$\gamma_2 = \frac{1-\gamma_1(N-\ell)}{\ell}. \tag{10}$$

Proof: First, we verify that ℓ_{min} can never be greater than $N-1$. It is sufficient to show that

$$\frac{\alpha-1}{\gamma_1} < N-1. \tag{11}$$

Eq. (11) is equivalent to stating $N > \alpha$, which is automatically fulfilled since $\alpha \in (1,N)$.

Now, consider $\ell \in \{\ell_{min}, \ell_{min}+1, ..., N-1\}$, and a fixed point $\mathbf{w} \in S^0_{N-1}$ of ISM having $N-\ell$ coordinates equal to γ_1. Then $\mathbf{w}$ has ℓ coordinates of value $\gamma_2 < N^{-1}$. Because $\mathbf{w} \in S^0_{N-1}$, we have

$$(N-\ell)\gamma_1 + \ell\gamma_2 = 1.$$

It follows that

$$\gamma_2 = \frac{1-\gamma_1(N-\ell)}{\ell}. \tag{12}$$

Note that γ_2 must be positive and so $\gamma_1 < (N-\ell)^{-1}$. This is indeed the case, since otherwise $\mathbf{w}$ would not lie in S^0_{N-1}.

Normalizing constant $Z(\mathbf{w};T)$ is equal to

$$Z(\mathbf{w};T) = (N-\ell)\cdot \exp\left(\frac{\gamma_1}{T}\right) + \ell \cdot \exp\left(\frac{\gamma_2}{T}\right).$$

Because $\mathbf{w}$ is a fixed point of ISM, we have

$$\gamma_1 = \frac{\exp\left(\frac{\gamma_1}{T}\right)}{Z(\mathbf{w};T)}.$$

Hence

$$\gamma_1 \cdot \left[(N-\ell) + \ell \exp\left(\frac{\gamma_2-\gamma_1}{T}\right)\right] = 1.$$

Consequently,

$$\gamma_1 \cdot \left[1 + \frac{\ell}{N-\ell}\exp\left(\frac{1-\alpha}{T\ell}\right)\right] = (N-\ell)^{-1}. \tag{13}$$

Equation (13) can be reformulated to

$$\exp\left(-\frac{\alpha-1}{T\ell}\right) = 1 - \frac{\alpha-1}{\ell\gamma_1}. \tag{14}$$

Since $\ell \geq \ell_{min} > (\alpha-1)/\gamma_1$, the right hand side of eq. (14) is always positive. Given the number ℓ of coordinates with value γ_2, we can solve for the temperature $T_e(\gamma_1;N,\ell)$ satisfying (14):

$$T_e(\gamma_1;N,\ell) = (\alpha-1)\left[-\ell \cdot \ln\left(1-\frac{\alpha-1}{\ell\gamma_1}\right)\right]^{-1}. \tag{15}$$

To conclude the proof, we need to show that γ_2 in eq. (12) satisfies the fixed point condition

$$\gamma_2 = \frac{\exp\left(\frac{\gamma_2}{T}\right)}{Z(\mathbf{w};T)}. \tag{16}$$

From (16) we have

$$\gamma_2 = \left[(N-\ell)\exp\left(\frac{\gamma_1-\gamma_2}{T}\right) + \ell\right]^{-1}.$$

Denote $(\gamma_1-\gamma_2)/T$ by ω. Then

$$\begin{aligned} \gamma_1 &= [N-\ell+\ell\exp(-\omega)]^{-1} \\ \gamma_2 &= [(N-\ell)\exp(\omega)+\ell]^{-1}. \end{aligned} \tag{17}$$

By (12),

$$\gamma_2 = \frac{1}{\ell}\left[1 - \frac{N-\ell}{N-\ell+\ell\exp(-\omega)}\right],$$

which reduces to (17).

By symmetry of the argument, there are $\binom{N}{\ell}$ possibilities for equilibria of ISM with $N-\ell$ and ℓ coordinates equal to γ_1 and γ_2, respectively. *Q.E.D.*

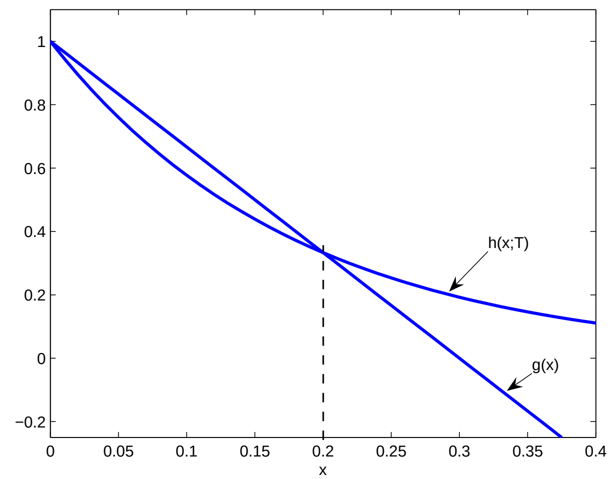

Figure 1: A geometric interpretation of the temperature $T_e(\gamma_1; N, \ell)$. The decreasing exponential function $h(x;T)$ is intersected by the decreasing line $g(x)$. Given a particular number ℓ, temperature T can be set to $T_e(\gamma_1; N, \ell)$, so that $h(x; T_e(\gamma_1; N, \ell))$ intersects $g(x)$ in $x_0 = \ell^{-1}$. In this case, $N = 10$, $\alpha = 1.5$, $\gamma_1 = 0.15$, $\ell_{min} = 4$, $\ell = 5$, $T_e(\gamma_1; N, \ell) = 0.0910$.

For a geometric interpretation of the temperature $T_e(\gamma_1; N, \ell)$, consider functions

$$h(x;T) = \exp\left(-\frac{\alpha - 1}{T}\, x\right) \quad \text{and} \tag{18}$$

$$g(x) = 1 - \frac{\alpha - 1}{\gamma_1}\, x, \tag{19}$$

operating on $(0, \infty)$ and plotted in figure 1. The decreasing exponential $h(x;T)$ is intersected by the decreasing line $g(x)$ at x_0. Given a particular number ℓ of coordinates of value γ_2, we can set T to $T = T_e(\gamma_1; N, \ell)$, so that the exponential $h(x; T_e(\gamma_1; N, \ell))$ intersects $g(x)$ in $x_0 = \ell^{-1}$.

Corollary 4.4 *Consider the ISM (7). For $\ell \in \{0, 1, ..., N-1\}$, define*

$$\alpha_\ell = \frac{N}{N - \ell}.$$

Fix $\alpha \in (1, N) \cup [\alpha_{\ell-1}, \alpha_\ell)$, $\ell \in \{1, ..., N-1\}$. Then, by varying the temperature parameter T, the ISM can have

$$Q_N(\alpha) = \sum_{k=\ell}^{N-1} \binom{N}{k}$$

distinct fixed points.

Proof: By Theorem 4.3, for $\alpha \in (1, N) \cup [\alpha_{\ell-1}, \alpha_\ell)$, there are temperature settings (9) so that points $\mathbf{w} \in S^0_{N-1}$ with $N-k$ and k coordinates equal to $\gamma_1 = \alpha N^{-1}$

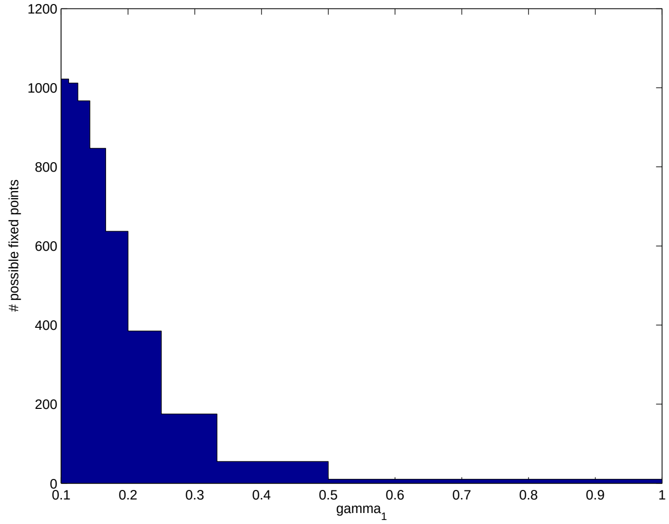

Figure 2: Number of possible fixed points as a function of the larger coordinate γ_1 in ISM with $N = 10$. The further we move from the maximum entropy equilibrium $\overline{\mathbf{w}} = (0.1, 0.1, ..., 0.1)'$, the less fixed points are possible.

and γ_2 (eq. (10)), respectively, are equilibria of the ISM, $k = \ell, \ell+1, ..., N-1$. For this value of α, no other fixed points are possible. This is easily observed, since for $\alpha \in (1, N) \cup [\alpha_{\ell-1}, \alpha_\ell)$, The lower bound ℓ_{min} on the number of smaller coordinates is equal to ℓ. *Q.E.D.*

Since $\alpha_0 = 1 < \alpha_1 < \alpha_2 < ... < \alpha_{N-1} = N$, Corollary 4.4 tells us that the richest structure of equilibria of ISM can be found in a small neighborhood of the maximum entropy fixed point $\overline{\mathbf{w}}$. The least number of fixed points exist in the "corner" areas of S_{N-1} ($\alpha_{N-2} = N/2 \leq \alpha < \alpha_{N-1} = N$), namely only $\binom{N}{N-1} = N$ fixed points are possible - points at the vertexes of S_{N-1}. In addition, we can analytically describe decreasing trend in the number of possible equilibria as one diverges from $\overline{\mathbf{w}}$. When increasing α crosses α_ℓ, the number of possible fixed points decreases by $\binom{N}{\ell}$. As an example we show in figure 2 the number of possible fixed points as a function of the larger coordinate γ_1 in a 10-dimensional ISM system.

5 Fixed point stability in Iterative Softmax

Lemma 5.1 *Let $\mathbf{w} \in S^0_{N-1}$, $\mathbf{w} \neq \overline{\mathbf{w}}$ be a fixed point of ISM with larger and smaller coordinates equal to γ_1 and γ_2, respectively. Then, γ_1 is never further from $\frac{1}{2}$ than γ_2 is; i.e.*

$$\left|\gamma_1 - \frac{1}{2}\right| \leq \left|\gamma_2 - \frac{1}{2}\right|. \tag{20}$$

Proof: Assume first that $\gamma_1 \in (0, \frac{1}{2}]$. Then since $\gamma_1 > \gamma_2$, (20) is automatically satisfied.

Assume now that $\gamma_1 \in (\frac{1}{2}, 1)$. Since $\mathbf{w} \in S^0_{N-1}$, there can be only one coordinate of $\mathbf{w}$ with value γ_1. Also $\gamma_2 < \frac{1}{2}$.

The coordinates must sum up to one, and so

$$\gamma_1 = 1 - (N-1)\gamma_2.$$

For $N \geq 2$ we have[4]

$$\left|\gamma_1 - \frac{1}{2}\right| = \gamma_1 - \frac{1}{2} = \frac{1}{2} - (N-1)\gamma_2 \leq \frac{1}{2} - \gamma_2 = \left|\gamma_2 - \frac{1}{2}\right|.$$

Q.E.D.

Theorem 5.2 *Consider a fixed point* $\mathbf{w} \in S^0_{N-1}$ *of ISM (7) with one of its coordinates equal to* $N^{-1} \leq \gamma_1 < 1$. *Then, if*

$$T > T_{s,1}(\gamma_1) = 2\ \gamma_1\ (1-\gamma_1), \tag{21}$$

or if

$$T > T_{s,2}(\gamma_1) = \gamma_1, \tag{22}$$

the fixed point $\mathbf{w}$ *is stable.*

Proof: Jacobian $J(\mathbf{w};T)$ of the ISM map (3)–(4), is given by (6). The Jacobian is a symmetric matrix and so the column and row sum norms coincide:

$$\|J(\mathbf{w};T)\|_\infty = \max_{i=1,2,\ldots,N} \left\{ \sum_{j=1}^{N} |J(\mathbf{w};T)_{i,j}| \right\}. \tag{23}$$

The sum of absolute values in the i-th row of the Jacobian is equal to

$$\begin{aligned}
\mathcal{S}_i &= \frac{F_i(\mathbf{w};T)}{T}\left[(1-F_i(\mathbf{w};T)) + \sum_{j\neq i} F_j(\mathbf{w};T)\right] && (24)\\
&= \frac{w_i}{T}\left[(1-w_i) + \sum_{j\neq i} w_j\right] && (25)\\
&= \frac{w_i}{T}\left[(1-w_i) + (1-w_i)\right] && (26)\\
&= \frac{2}{T} w_i (1-w_i). && (27)
\end{aligned}$$

Note that (25) follows form (24) because $\mathbf{w}$ is a fixed point of $\mathbf{F}$, i.e. $\mathbf{w} = \mathbf{F}(\mathbf{w})$, and (26) follows form (25) because $\mathbf{w} \in S^0_{N-1}$. We have

$$\begin{aligned}
\|J(\mathbf{w};T)\|_\infty &= \max_{i=1,2,\ldots,N} \{\mathcal{S}_i\} && (28)\\
&= \frac{2}{T} \max_{i=1,2,\ldots,N} \{q(w_i)\}, && (29)
\end{aligned}$$

[4] recall that we study systems for $N \geq 2$

where $q : [0,1] \to [0,1/4]$ is a unimodal function $q(x) = x(1-x)$ with maximum at $x = 1/2$. Point $x = 1/2$ is also the point of symmetry. Hence,

$$\|J(\mathbf{w};T)\|_\infty = \frac{2}{T} q(\tilde{w}),$$

where $\tilde{w}$ is the coordinate value of $\mathbf{w}$ closest to $1/2$.

By theorem 4.2, there can be at most two distinct values taken on by the coordinates of $\mathbf{w}$. If $\mathbf{w} = \overline{\mathbf{w}}$, all the coordinates are the same and $\tilde{w} = N^{-1}$. If $\mathbf{w} \neq \overline{\mathbf{w}}$, by lemma 5.1, it is the bigger value of the two[5], $\gamma_1 > N^{-1}$, that is close to $1/2$. Hence $\tilde{w} = \gamma_1$. It follows that if one of the coordinates of $\mathbf{w}$ is equal to $N^{-1} \leq \gamma_1 < 1$, then $\|J(\mathbf{w};T)\|_\infty = 2q(\gamma_1)/T$.

Now, if $\|J(\mathbf{w};T)\|_\infty < 1$, the fixed point $\mathbf{w}$ is contractive. In other words, if $T > T_{s,1}(\gamma_1) = 2\gamma_1(1-\gamma_1)$, $\mathbf{w}$ is a stable fixed point of ISM (7).

Note that all eigenvalues of Jacobian $J(\mathbf{w};1)$ (ISM operating at temperature 1) are upper-bounded by $\max_{1 \leq k \leq N} F_k(\mathbf{w};1)$ (Elfadel and Wyatt, 1994). It follows that all eigenvalues of $J(\mathbf{w};T)$ are upper-bounded by $\max_{1 \leq k \leq N} T^{-1}\ F_k(\mathbf{w};T)$. For each fixed point $\mathbf{w}$ of ISM operating at temperature T, $\mathbf{w} = \mathbf{F}(\mathbf{w};T)$ and so by theorem 4.2, all eigenvalues of $J(\mathbf{w};T)$ are upper-bounded by $\gamma_1 T^{-1}$. Hence, the spectral radius $\rho(J(\mathbf{w};T))$ of $J(\mathbf{w};T)$ (the maximal absolute value of eigenvalues of $J(\mathbf{w};T)$) is upper-bounded by $\gamma_1 T^{-1}$. If $\rho(J(\mathbf{w};T)) < 1$, i.e. if $T > T_{s,2}(\gamma_1) = \gamma_1$, $\mathbf{w}$ is a stable equilibrium of ISM (7). *Q.E.D.*

Since $T_{s,2}(\gamma_1) \leq T_{s,1}(\gamma_1)$ on $(N^{-1}, 1/2]$ and $T_{s,2}(\gamma_1) > T_{s,1}(\gamma_1)$ on $(1/2, 1)$, it is useful to combine the two bounds into a single one.

Corollary 5.3 *Consider a fixed point $\mathbf{w} \in S^0_{N-1}$ of ISM (7) with one of its coordinates equal to $N^{-1} \leq \gamma_1 < 1$. Define*

$$T_s(\gamma_1) = \begin{cases} T_{s,2}(\gamma_1), & \text{if } \gamma_1 \in [N^{-1}, 1/2) \\ T_{s,1}(\gamma_1), & \text{if } \gamma_1 \in [1/2, 1). \end{cases} \tag{30}$$

Then, if $T > T_s(\gamma_1)$, the fixed point $\mathbf{w}$ is stable.

Lemma 4.1 tells us that the maximum entropy point $\overline{\mathbf{w}} = (N^{-1}, N^{-1}, ..., N^{-1})'$ is an equilibrium of ISM (7) for any temperature setting T. By theorem 5.2, for $T > T_s(N^{-1}) = N^{-1}$, $\overline{\mathbf{w}}$ is guaranteed to be stable. The next theorem claims that for high temperature settings, no fixed points other than $\overline{\mathbf{w}}$ exist, i.e. $\overline{\mathbf{w}}$ is the unique equilibrium of ISM.

Theorem 5.4 *For $T > 1/2$, the maximum entropy point $\overline{\mathbf{w}} = (N^{-1}, N^{-1}, ..., N^{-1})'$ is the unique equilibrium of ISM (7).*

[5] note that the smaller value γ_2 is automatically less than N^{-1}

Proof: For any $\mathbf{w} \in S^0_{N-1}$,

$$
\begin{aligned}
\|J(\mathbf{w};T)\|_\infty &= \max_{i=1,2,\ldots,N} \frac{F_i(\mathbf{w};T)}{T}\left[(1-F_i(\mathbf{w};T)) + \sum_{j\neq i} F_j(\mathbf{w};T)\right] \\
&= \max_{i=1,2,\ldots,N} \frac{2}{T}\left[F_i(\mathbf{w};T)(1-F_i(\mathbf{w};T))\right] \\
&\leq \frac{2}{T}\frac{1}{4} = \frac{1}{2T}.
\end{aligned} \tag{31}
$$

For $T > 1/2$, the ISM (7) is a global contraction. By the Banach fixed point theorem, there exists a unique attractive fixed point of the ISM. But $\overline{\mathbf{w}}$ is always a fixed point of the ISM. It follows that for $T > 1/2$, the only fixed point of ISM (7) is $\overline{\mathbf{w}}$. In addition, $\overline{\mathbf{w}}$ is attractive. *Q.E.D.*

Theorem 5.4 sharpens the statement by Elfadel and Wyatt (1994) that points of S_{N-1} converge under ISM (7) to $\overline{\mathbf{w}}$ as $T \to \infty$.

We now turn our attention to conditions under which fixed points of ISM are not stable.

Theorem 5.5 *Consider a fixed point $\mathbf{w} \in S^0_{N-1}$ of ISM (7) with one of its coordinates equal to $N^{-1} \leq \gamma_1 < 1$. Let $N-\ell$ be the number of coordinates of value γ_1. Then if*

$$
T < T_u(\gamma_1; N, \ell) = \gamma_1\ (2 - N\gamma_1)\frac{N-\ell}{N\ell} + \frac{1}{N} - \frac{1}{N\ell}, \tag{32}
$$

$\mathbf{w}$ *is not stable.*

Proof: Let $\rho(J(\mathbf{w};T))$ be the spectral radius of the Jacobian $J(\mathbf{w};T)$. If for a fixed point $\mathbf{w}$ of ISM (7) $\rho(J(\mathbf{w};T)) > 1$, the fixed point is not stable.

Note that

$$
\rho(J(\mathbf{w};T)) \geq \frac{1}{N}\sum_{i=1}^{N}|\lambda_i| \geq \frac{1}{N}\left|\sum_{i=1}^{N}\lambda_i\right| = \frac{|\mathrm{trace}(J(\mathbf{w};T))|}{N},
$$

where λ_i are eigenvalues of the Jacobian $J(\mathbf{w};T)$. By Theorem 4.3, $\mathbf{w} \in S^0_{N-1}$ has to have ℓ coordinates equal to

$$
\gamma_2 = \frac{1-\gamma_1(N-\ell)}{\ell}.
$$

We have

$$
\begin{aligned}
|\mathrm{trace}(J(\mathbf{w};T))| &= \frac{1}{T}[(N-\ell)\gamma_1(1-\gamma_1) + \ell\gamma_2(1-\gamma_2)] \\
&= \frac{1}{\ell T}\left[\gamma_1\ (2-N\gamma_1)(N-\ell) + \ell - 1\right].
\end{aligned}
$$

The result follows by imposing

$$\frac{|\mathrm{trace}(J(\mathbf{w};T))|}{N} > 1.$$

Q.E.D.

Note that by theorem 5.5, for temperatures

$$T < T_u(N^{-1};N,N) = N^{-1} - N^{-2} = T_s(N^{-1}) - N^{-2},$$

the maximum entropy equilibrium $\overline{\mathbf{w}}$ of ISM (7) cannot be attractive. This bound can be further improved by realizing that the Jacobian $J(\overline{\mathbf{w}};T)$ (6) of ISM (7) at $\overline{\mathbf{w}}$ has exactly one zero eigenvalue (corresponding to the eigenvector $(1,1,...,1)'$) and $N-1$ eigenvalues equal to $(NT)^{-1}$. Hence the spectral radius is equal to

$$\rho(J(\overline{\mathbf{w}};T)) = \frac{1}{NT}. \tag{33}$$

It follows that the maximum entropy equilibrium $\overline{\mathbf{w}}$ is attractive and non-attractive if $T > N^{-1}$ and $T < N^{-1}$, respectively.

An illustrative summary of the previous results for equilibria $\mathbf{w} \neq \overline{\mathbf{w}}$ is provided in figure 3. The ISM has $N = 10$ units. Coordinates of such fixed points can only take on two possible values, the larger of which we denote by γ_1. Temperatures $T_s(\gamma_1)$ (30) above which equilibria with larger coordinate equal to γ_1 are guaranteed to be stable are shown as the solid bold line. Denote the number of coordinates with value γ_1 by N_1, i.e. $N_1 = N - \ell$. For $N_1 = 1,2,3,4$, we show temperatures $T_u(\gamma_1;N,\ell)$ (32) below which equilibria with larger coordinate equal to γ_1 are guaranteed to be unstable with solid normal lines[6]. For a given value of γ_1, temperatures between $T_u(\gamma_1;N,\ell)$ and $T_s(\gamma_1)$ potentially correspond to saddle-type equilibria. We also plot temperatures $T_e(\gamma_1;N,\ell)$ (9) at which equilibria with the given number N_1 of coordinates of value γ_1 exist (dashed lines). The figure suggests that most of ISM equilibria with more than one larger coordinate γ_1, i.e. $N_1 \geq 2$, are of saddle type. Only fixed points with extreme values of γ_1 close to N_1^{-1} are guaranteed to be unstable. These findings were numerically confirmed by eigenvalue decomposition of Jacobians of a large number of fixed points corresponding to the dashed lines. Note that, apart from the maximum entropy equilibrium $\overline{\mathbf{w}}$, only the "extreme" equilibria close to the vertexes of simplex S_{N-1} can be guaranteed by our theory to be stable. This happens when the dashed line for $N_1 = 1$ crosses the solid bold line.

We now show that the character of the partitioning of the (γ_1, T)-space with respect to stability regimes of ISM equilibria remains unchanged for other values of N (dimensionality of ISM).

Lemma 5.6 *Consider equilibria of an N-dimensional ($N > 2$) ISM (7) with at least two larger coordinates of value γ_1, i.e. $\ell \leq N-2$ and $\gamma_1 \in (N^{-1},(N-\ell)^{-1})$. Then,*

[6] note that since $\mathbf{w} \in S^0_{N-1}$, γ_1 must be smaller than $1/N_1$

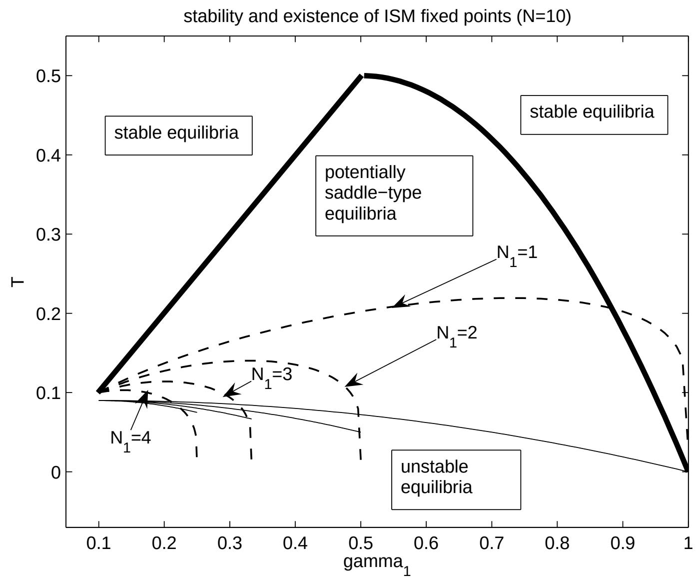

Figure 3: Stability regions for equilibria $\mathbf{w} \neq \overline{\mathbf{w}}$ of ISM with $N = 10$ units as a function of the larger coordinate γ_1 and temperature T. The number of coordinates with value γ_1 is denoted by N_1. Temperatures $T_s(\gamma_1)$ (30) above which equilibria with larger coordinate equal to γ_1 are guaranteed to be stable are shown with solid bold line. For $N_1 = N - \ell \in \{1, 2, 3, 4\}$, we show the temperatures $T_u(\gamma_1; N, \ell)$ (32) below which equilibria with larger coordinate equal to γ_1 are guaranteed to be unstable with solid normal lines. Also plotted are temperatures $T_e(\gamma_1; N, \ell)$ (9) at which equilibria with the given number N_1 of coordinates of value γ_1 exist (dashed lines).

for the temperature function (9),

$$T_{\ell,N}(\gamma_1) = T_e(\gamma_1; N, \ell) = (N\gamma_1 - 1)\left[\ell \cdot \ln\left(\frac{\ell\gamma_1}{\gamma_1(\ell - N) + 1}\right)\right]^{-1}, \tag{34}$$

guaranteeing the existence of such equilibria, it holds:

1. $T_{\ell,N}(N^{-1}) = T_s(N^{-1})$,
2. $T_{\ell,N}$ *is concave.*
3. $T'_{\ell,N}(N^{-1}) = 1 - N/(2\ell)$.

Proof:

1. At $\gamma_1 = 1/N$, both the numerator and denominator of (34) are zero. By L'Hospital rule[7]

$$\lim_{\gamma_1 \to N^{-1}} T_{\ell,N}(\gamma_1) = \lim_{\gamma_1 \to N^{-1}} \frac{N\gamma_1[\gamma_1(\ell - N) + 1]}{\ell} = \frac{1}{N} = T_s(N^{-1}). \tag{35}$$

2. The first derivative of $T_{\ell,N}$ is calculated as

$$T'_{\ell,N}(\gamma_1) = \frac{N}{\ell \ln\left(\frac{\ell\gamma_1}{\gamma_1(\ell-N)+1}\right)} - \frac{N\gamma_1 - 1}{\ell \ln^2\left(\frac{\ell\gamma_1}{\gamma_1(\ell-N)+1}\right)[\gamma_1^2(\ell - N) + \gamma_1]}. \tag{36}$$

To ease the presentation, $\ln(\cdot)$ will stand for $\ln\left(\frac{\ell\gamma_1}{\gamma_1(\ell-N)+1}\right)$. We write $T'_{\ell,N}(\gamma_1) = \ell^{-1}(A(\gamma_1) - B(\gamma_1))$, where

$$A(\gamma_1) = \frac{N}{\ln(\cdot)}$$

and

$$B(\gamma_1) = \frac{N\gamma_1 - 1}{\ln(\cdot)^2\gamma_1[\gamma_1(\ell - N) + 1]}.$$

Derivative of $A(\gamma_1)$,

$$A'(\gamma_1) = -\frac{N}{\ln(\cdot)^2\gamma_1[\gamma_1(\ell - N) + 1]},$$

is negative, as for $\gamma_1 \in (N^{-1}, (N - \ell)^{-1})$, we have $\gamma_1(\ell - N) + 1 > 0$.

Denote $\ln(\cdot)^2\gamma_1[\gamma_1(\ell - N) + 1]$ by C. Then,

$$B'(\gamma_1) = C^{-2}(D(\gamma_1)\ln(\cdot)^2 + 2\ln(\cdot)),$$

where

$$D(\gamma_1) = N(N - \ell)\gamma_1^2 - 2(N - \ell)\gamma_1 + 1.$$

[7] we slightly abuse mathematical notation by considering γ_1 continuous variable

Now, $D(\gamma_1)$ is a convex function with minimum at N^{-1} and $D(N^{-1}) = \ell/N > 0$. Also note that since $\gamma_1 > N^{-1}$, we have

$$\frac{\ell\gamma_1}{\gamma_1(\ell - N) + 1} > 1$$

and so $\ln(\cdot) > 0$.

From $A'(\gamma_1) < 0$ and $B'(\gamma_1) > 0$, it follows that $T''_{\ell,N}(\gamma_1) < 0$ and $T_{\ell,N}$ is concave.

3. The result follows from evaluation of $\lim_{\gamma_1 \to N^{-1}} T'_{\ell,N}(\gamma_1)$ based on (36). After applying L'Hospital rule twice, we get

$$\lim_{\gamma_1 \to N^{-1}} T'_{\ell,N}(\gamma_1) = 1 - \frac{N}{2\ell}.$$

Q.E.D.

We are now ready to prove that for equilibria of ISM (7) with at least two larger coordinates $\gamma_1 > N^{-1}$, the temperatures at which they exist, $T_e(\gamma_1; N, \ell)$, are always below the bound $T_s(\gamma_1)$, above which their stability is guaranteed.

Theorem 5.7 *Let $N > 2$ and $\ell \leq N - 2$. Then, for $\gamma_1 \in (N^{-1}, (N-\ell)^{-1})$, it holds:*

$$T_e(\gamma_1; N, \ell) < T_s(\gamma_1).$$

Proof: By lemma 5.6 (2), $T_{\ell,N}(\gamma_1) = T_e(\gamma_1; N, \ell)$ is a concave function and hence can be upper-bounded on $(N^{-1}, (N-\ell)^{-1})$ by the tangent line $\kappa(\gamma_1)$ to $T_{\ell,N}(\gamma_1)$ at N^{-1}:

$$T_{\ell,N}(\gamma_1) \leq \kappa(\gamma_1),$$

where by (35) and lemma 5.6 (1,3),

$$\kappa(\gamma_1) = \frac{1}{N} + \left(1 - \frac{N}{2\ell}\right)\left(\gamma_1 - \frac{1}{N}\right).$$

Now, $T_s(\gamma_1)$ is a line,

$$T_s(\gamma_1) = \frac{1}{N} + \left(\gamma_1 - \frac{1}{N}\right).$$

Since $N/(2\ell) > 0$, we have that on $(N^{-1}, (N-\ell)^{-1})$, $T_e(\gamma_1; N, \ell) < T_s(\gamma_1)$. Hence, the tangent $\kappa(\gamma_1)$ upper-bounding $T_s(\gamma_1)$ never crosses $T_s(\gamma_1)$ and always stays below it. *Q.E.D.*

As an illustrative example, we present analog of figure 3 for 17-dimensional ISM in figure 4. The number of coordinates with value γ_1 is denoted by N_1. Temperatures

$T_s(\gamma_1)$ (30) above which equilibria with larger coordinate equal to γ_1 are guaranteed to be stable are shown with solid bold line. For $N_1 = N - \ell \in \{1, 2, 3, 4\}$, we show the temperatures $T_u(\gamma_1; N, \ell)$ (32) below which equilibria with larger coordinate equal to γ_1 are guaranteed to be unstable with solid normal lines. Temperatures $T_e(\gamma_1; N, \ell)$ (9) at which equilibria with the given number N_1 of coordinates of value γ_1 exist (dashed lines) are also marked according to stability type of the corresponding fixed points. The stability types were determined by eignanalysis of Jacobians (6) at the fixed points. Stable and unstable equilibria existing at temperature $T_e(\gamma_1; N, \ell)$ are shown as stars and circles, respectively. All the unstable equilibria are of saddle type. Horizontal dashed line shows a numerically determined temperature by Kwok and Smith (2005) at which attractive equilibria of 17-dimensional ISM lose stability and the maximum entropy point $\overline{\mathbf{w}}$ remains the only stable fixed point. Position where $T_s(\gamma_1)$ crosses $T_e(\gamma_1; N, \ell)$ for $N_1 = 1$ is marked by bold circle. Note that no equilibrium with more than one coordinate greater than N^{-1} is stable.

6 Critical temperature for intermittent search in SONN with softmax weight renormalization

It has been hypothesized that ISM provides an underlying driving force behind intermittent search in SONN with softmax weight renormalization (Kwok and Smith, 2003, 2005) (see section 2). Kwok and Smith (2005) argue that the critical temperature at which the intermittent search takes place corresponds to the "bifurcation point" of the *autonomous* ISM dynamics when the existing equilibria lose stability and only the maximum entropy point $\overline{\mathbf{w}}$ survives as the sole stable equilibrium. The authors numerically determined such bifurcation points for several ISM dimensionalities N. It was reported that bifurcation temperatures decreased with increasing N. Based on the analysis in section 5, the bifurcation points correspond to the case when equilibria near corners of the simplex S_{N-1} (equilibria with only one coordinate with large value γ_1) lose stability. Based on the bound $T_s(\gamma_1)$ (30) and temperatures $T_e(\gamma_1; N, N-1)$ (9) at which equilibria of ISM exist, such a bifurcation point can be approximated by a bold circle in figure 4. Figure 5 shows evolution of the approximation of the bifurcation point (based on $T_e(\gamma_1; N, N-1)$ (9) and bound $T_s(\gamma_1)$ (30)) for increasing ISM dimensionalities N. The bound (30) is independent of N. In accordance with empirical findings of Kwok and Smith, the bifurcation temperature is decreasing with increasing N.

We present two approximations to the critical temperature $T_*(N)$ at which the bifurcation occurs. The first one expands $T_e(\gamma_1; N, N-1)$ (9) around γ_1^0 as a second-order polynomial $T^{(2)}_{N-1}(\gamma_1)$. Based on figure 5, a good choice for γ_1^0 is e.g. $\gamma_1^0 = 0.9$. Approximation to the critical temperature is then obtained by solving

$$T^{(2)}_{N-1}(\gamma_1) = T_s(\gamma_1)$$

for $\gamma_1 = \alpha/N$, and then plugging the solution $\gamma_1^{(2)}$ back to bound (30), i.e. calculating $T_s(\gamma_1^{(2)})$.

We have

$$T_e(\gamma_1; N, N-1) = \frac{N\gamma_1 - 1}{(N-1)\ln\left(\frac{(N-1)\gamma_1}{1-\gamma_1}\right)}, \tag{37}$$

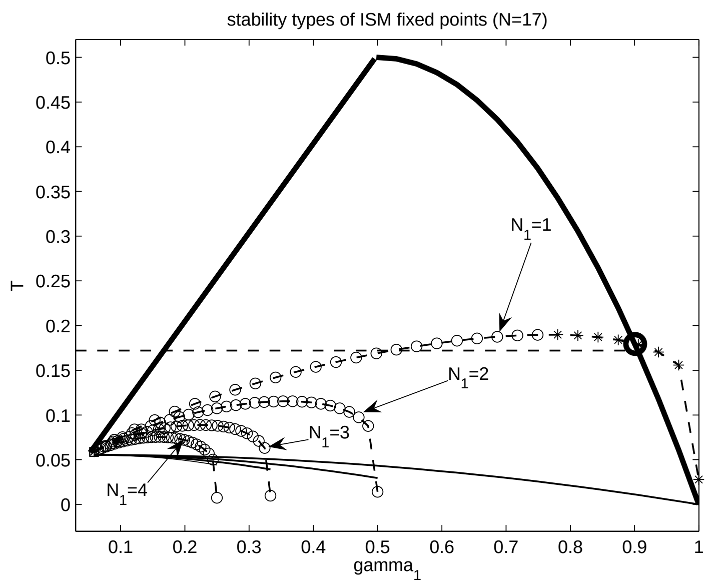

Figure 4: Stability types for equilibria $\mathbf{w} \neq \overline{\mathbf{w}}$ of ISM with $N = 17$ units as a function of the larger coordinate γ_1 and temperature T. The number of coordinates with value γ_1 is denoted by N_1. Temperatures $T_s(\gamma_1)$ (30) above which equilibria with larger coordinate equal to γ_1 are guaranteed to be stable are shown with solid bold line. For $N_1 = N - \ell \in \{1, 2, 3, 4\}$, we show the temperatures $T_u(\gamma_1; N, \ell)$ (32) below which equilibria with larger coordinate equal to γ_1 are guaranteed to be unstable with solid normal lines. Temperatures $T_e(\gamma_1; N, \ell)$ (9) at which equilibria with the given number N_1 of coordinates of value γ_1 exist (dashed lines) are also marked according to the stability type of the corresponding fixed points. Stable and unstable equilibria existing at temperature $T_e(\gamma_1; N, \ell)$ are shown as stars and circles, respectively. Horizontal dashed line shows a numerically determined temperature by Kwok and Smith (2005) at which attractive equilibria of 17-dimensional ISM lose stability and the maximum entropy point $\overline{\mathbf{w}}$ remains the only stable fixed point. Bold circle marks the position where $T_s(\gamma_1)$ crosses $T_e(\gamma_1; N, \ell)$ for $N_1 = 1$.

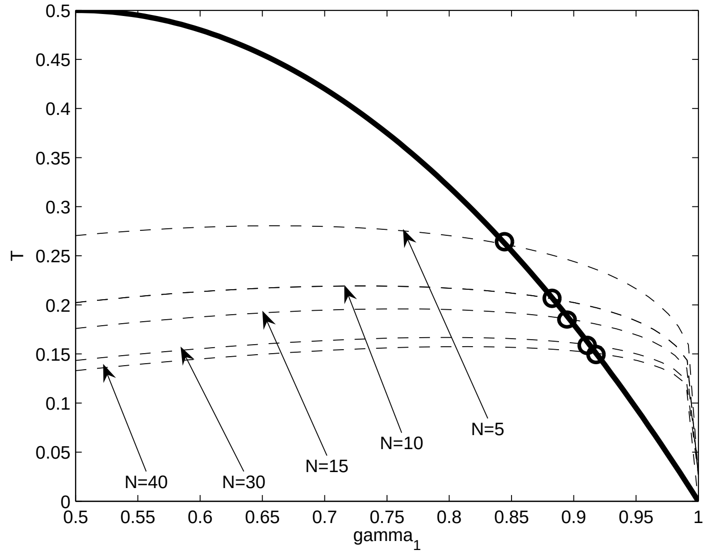

Figure 5: Approximations of the bifurcation point based on (9) and bound (30) for increasing ISM dimensionalities N.

$$T_e'(\gamma_1; N, N-1) = \frac{N}{(N-1)\ln\left(\frac{(N-1)\gamma_1}{1-\gamma_1}\right)} - \frac{N\gamma_1 - 1}{(N-1)\gamma_1(1-\gamma_1)\ln^2\left(\frac{(N-1)\gamma_1}{1-\gamma_1}\right)} \tag{38}$$

and

$$T_e''(\gamma_1; N, N-1) = \frac{N\gamma_1^2 - 2\gamma_1 + 1 - 2\ln^{-1}\left(\frac{(N-1)\gamma_1}{1-\gamma_1}\right)}{(N-1)\gamma_1^2(1-\gamma_1)^2\ln^2\left(\frac{(N-1)\gamma_1}{1-\gamma_1}\right)}. \tag{39}$$

By solving

$$A\gamma_1^2 + B\gamma_1 + C = 0, \tag{40}$$

where

$$A = \frac{1}{2}T_e''(\gamma_1^0; N, N-1) + 2,$$
$$B = T_e'(\gamma_1^0; N, N-1) - \gamma_1^0\ T_e''(\gamma_1^0; N, N-1) - 2,$$
$$C = T_e(\gamma_1^0; N, N-1) - \gamma_1^0\ T_e'(\gamma_1^0; N, N-1) + \frac{1}{2}(\gamma_1^0)^2\ T_e''(\gamma_1^0; N, N-1)$$

and retaining the solution $\gamma_1^{(2)}$ compatible with the requirement that $\mathbf{w} \in S_{N-1}$, we obtain an analytical approximation $T_*^{(2)}(N)$ to the critical temperature $T_*(N)$:

$$T_*^{(2)}(N) = 2\gamma_1^{(2)}(1 - \gamma_1^{(2)}). \tag{41}$$

A cheaper approximation to $T_*(N)$ can be obtained by realizing that both functions in figure 5 are almost linear in the neighborhood of their intersection. First we approximate the bound $T_s(\gamma_1)$ (30) (solid bold line) by the tangent line at (1,0):

$$v(\gamma_1) = 2(1 - \gamma_1). \tag{42}$$

Imposing $v(\gamma_1) = T_e(\gamma_1; N, N-1)$ leads to

$$y = 2(N-1)\ln(y) - 1, \tag{43}$$

where

$$y = \frac{(N-1)\gamma_1}{1-\gamma_1}. \tag{44}$$

We expand the RHS of (43) around y^0 (corresponding to γ_1^0) as

$$\frac{2(N-1)}{y^0} y + 2(N-1)(1 + \ln(y^0)) - 1$$

and so the approximate solution to (43) reads

$$y^{(1)} = \frac{2(N-1)(1 + \ln(y^0)) - 1}{1 - \frac{2(N-1)}{y^0}}. \tag{45}$$

From (44), the corresponding value of γ_1 is

$$\gamma_1^{(1)} = \frac{y^{(1)}}{N - 1 + y^{(1)}}, \tag{46}$$

yielding an approximation $T_*^{(1)}(N)$ to the critical temperature $T_*(N)$:

$$T_*^{(1)}(N) = 2\gamma_1^{(1)}(1 - \gamma_1^{(1)}). \tag{47}$$

To illustrate the approximations $T_*^{(1)}(N)$ and $T_*^{(2)}(N)$ of the critical temperature $T_B = T_*(N)$, numerically found bifurcation temperatures for ISM systems with dimensions between 8 and 30 are shown in figure 6 as circles. The approximations based on quadratic and linear expansions, $T_*^{(2)}(N)$ and $T_*^{(1)}(N)$, are plotted with bold solid and dashed lines, respectively. Also shown are the temperatures $1/N$ above which the maximum entropy equilibrium $\overline{\mathbf{w}}$ is stable (solid normal line). At bifurcation temperature, $\overline{\mathbf{w}}$ is already stable and equilibria at vertexes of simplex S_{N-1} lose stability. The analytical solutions $T_*^{(2)}(N)$ and $T_*^{(1)}(N)$ appear to approximate the bifurcation temperatures well.

We also numerically determined optimal temperature settings for intermittent search by SONN in the N-queens problems. Following (Kwok and Smith, 2005), the SONN parameter β was set to $\beta = 0.8$[8]. The optimal neighborhood size increased with the problem size N from $L = 2$ (for $N = 8$), through $L = 3$ ($N = 10, 13$), $L = 4$ ($N = 15, 17, 20$), to $L = 5$ ($N = 25, 30$)[9]. Based on our extensive experimentation, the best performing temperatures for intermittent search in the N-queens problems are shown as stars. Clearly, as suggested by Kwok and Smith, there is a marked correspondence between the bifurcation temperatures of ISM equilibria and the best performing temperatures in intermittent search by SONN.

[8]Our experiments confirmed finding by Kwok and Smith that the choice of β is in general not sensitive to N.

[9]the increase of optimal neighborhood size L with increasing problem dimension N is in accordance with findings in (Kwok and Smith, 2005)

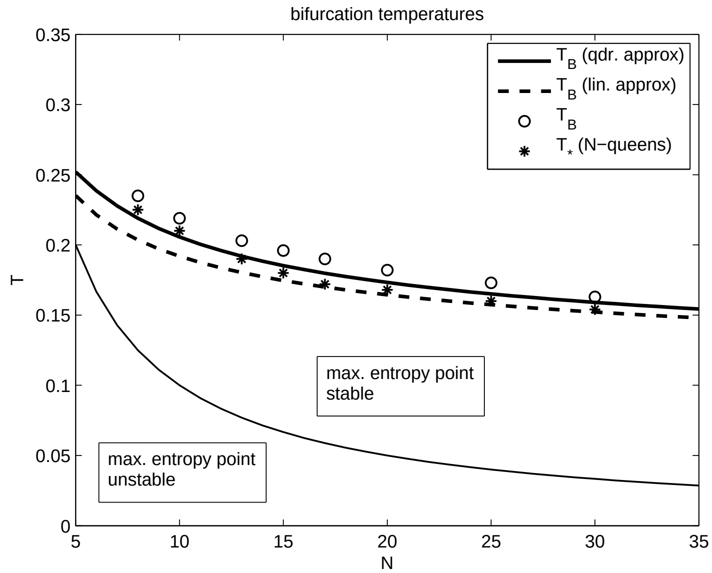

Figure 6: Analytical approximations of the bifurcation temperature $T_B = T_*(N)$ for increasing ISM dimensionalities N. The approximations based on quadratic and linear expansions, $T_*^{(2)}(N)$ and $T_*^{(1)}(N)$, are plotted with bold solid and dashed lines, respectively. Numerically found bifurcation temperatures are shown as circles. The best performing temperatures for intermittent search in the N-queens problems are shown as stars. Also shown are the temperatures $1/N$ above which the maximum entropy equilibrium $\overline{\mathbf{w}}$ is stable. As suggested by Kwok and Smith, there is a marked correspondence between the bifurcation temperatures and the best performing temperatures in intermittent search by SONN. The analytical solutions $T_*^{(2)}(N)$ and $T_*^{(1)}(N)$ appear to approximate the bifurcation temperatures well.

The only equilibria that can be guaranteed to be stable by our theory are the maximum entropy point $\overline{\mathbf{w}}$ and "one-hot" solutions at the vertexes of the $N-1$ dimensional simplex S_{N-1}. Each of such "one-hot" solutions corresponds to one particular assignment of SONN inputs to SONN outputs. At the critical point of loosing their stability, the "one-hot" solutions do not exhibit a strong attractive force in the ISM state space and SONN weight updates can easily jump from one assignment to another, occasionally being pulled by the neutralizing power of the stable maximum entropy equilibrium $\overline{\mathbf{w}}$. This mechanism enables rapid intermittent search for good assignment solutions in SONN. Obviously, much more work is needed to rigorously analyze the intricate influence of the neighborhood size, SONN weight updates and softmax renormalization in a unified framework. This is a matter of our future work. It is highly encouraging, however, that the *analytically* obtained approximations of critical temperatures predict the optimal working temperatures for SONN intermittent search very well. So far the critical temperatures have been determined only via extensive trial-and-error numerical investigations.

Note that, as a direct consequence of theorem 5.4, no intermittent search can exist in SONN for temperatures $T > 1/2$.

7 Conclusions

Recently proposed new kind of optimization dynamics using self-organizing neural networks driven by softmax weight renormalization is capable of powerful intermittent search for high-quality solutions in difficult assignment optimization problems (Kwok and Smith, 2005). However, such dynamics is sensitive to temperature setting in the softmax renormalization step. It has been hypothesized by Kwok and Smith (2005) that the optimal temperature setting corresponds to symmetry breaking bifurcation of equilibria of the renormalization step, when viewed as an autonomous dynamical system. Following (Kwok and Smith, 2003, 2005), we call such dynamical systems iterative softmax (ISM).

We have rigorously analyzed equilibria of ISM. In particular, we determined their number, position and stability types. Most fixed points can be found in the neighborhood of the maximum entropy equilibrium point $\overline{\mathbf{w}} = (N^{-1}, N^{-1}, ..., N^{-1})'$. We have calculated the exact rate of decrease in the number of ISM equilibria as one moves away from $\overline{\mathbf{w}}$. We have derived bounds on temperatures guaranteeing different stability types of ISM equilibria. It appears that most of ISM fixed points are of saddle type. This hypothesis is supported by our extensive numerical experiments[10].

The only equilibria that can be guaranteed to be stable by our theory are the maximum entropy point $\overline{\mathbf{w}}$ and "one-hot" solutions at the vertexes of the $N-1$ dimensional simplex. We argued that close to the critical bifurcation temperature at which such "one-hot" equilibria lose stability the most powerful intermittent search can take place in SONN. Based on temperature bounds guaranteeing stability of "one-hot" equilibria and temperatures guaranteeing their existence, we were able to derive *analytical* approximations to the critical bifurcation temperatures that are in good agreement with those found by numerical investigations. So far the critical temperatures have been determined only via extensive trial-and-error numerical investigations. Moreover, the analytically obtained critical temperatures predict the optimal working temperatures for SONN intermittent search very well. We have also shown that no intermittent search can exist in SONN for temperatures greater than 1/2.

References

J.P. Crutchfield and K. Young. Computation at the onset of chaos. In W.H. Zurek, editor, *Complexity, Entropy, and the physics of Information, SFI Studies in the Sciences of Complexity, vol 8*, pages 223–269. Addison-Wesley, 1990.

I.M. Elfadel and J.L. Wyatt. The softmax nonlinearity: Derivation using statistical mechanics and useful properties as a multiterminal analog circuit element. In J. Cowan, G. Tesauro, and C.L. Giles, editors, *Advances in Neural Information Processing Systems 6*, pages 882–887. Morgan Kaufmann, 1994.

S. Gold and A. Rangarajan. Softmax to softassign: Neural network algorithms for combinatorial optimization, 1996.

[10] most of them are not reported here

F. Guerrero, S. Lozano, K.A. Smith, D. Canca, and T. Kwok. Manufacturing cell formation using a new self-organizing neural network. *Computers & Industrial Engineering*, 42:377–382, 2002.

J.J. Hopfield. Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the National Academy of Science USA*, 79: 2554–2558, 1982.

T. Kohonen. Self–organizing formation of topologically correct feature maps. *Biological Cybernetics*, 43:59–69, 1982.

J.J. Kosowsky and A.L. Yuille. The invisible hand algorithm: Solving the assignment problem with statistical physics. *Neural Networks*, 7(3):477–490, 1994.

T. Kwok and K.A. Smith. Characteristic updating-normalisation dynamics of a self-organising neural network for enhanced combinatorial optimisation. In *Proceedings of the 9th International Conference on Neural Information Processing (ICONIP'2002)*, volume 3, pages 1146–1152, Singapore, 2002.

T. Kwok and K.A. Smith. Performance-enhancing bifurcations in a self-organising neural network. In *Computational Methods in Neural Modeling: Proceedings of the 7th International Work-Conference on Artificial and Natural Neural Networks (IWANN'2003)*, volume Lecture Notes in Computer Science, vol. 2686, pages 390–397, Singapore, 2003. Springer-Verlag, Berlin.

T. Kwok and K.A. Smith. A noisy self-organizing neural network with bifurcation dynamics for combinatorial optimization. *IEEE Transactions on Neural Networks*, 15(1):84–88, 2004.

T. Kwok and K.A. Smith. Optimization via intermittency with a self-organizing neural network. *Neural Computation*, 17:2454–2481, 2005.

C.G. Langton. Computation at the edge of chaos: Phase transitions and emergent computation. *Physica D*, 42:12–37, 1990.

S. Minton, M.D. Johnston, A.B. Philips, and P. Laird. Minimizing conflicts: A heuristic repair method for constraint satisfaction and scheduling problems. *Artificial Intelligence*, 58(1-3):161–205, 1992.

A. Rangarajan. Self-annealing and self-annihilation: unifying deterministic annealing and relaxation labeling. *Pattern Recognition*, 33(4):635–649, 2000.

K.A. Smith. Solving the generalized quadratic assignment problem using a self-organizing process. In *Proceedings of the IEEE Int. Conf. on Neural Networks*, volume 4, pages 1876–1879, 1995.

K.A. Smith. Neural networks for combinatorial optimization: a review of more than a decade of research. *INFORMS Journal on Computing*, 11(1):15–34, 1999.

K.A. Smith, M. Palaniswami, and M. Krishnamoorthy. Neural techniques for combinatorial optimization with applications. *IEEE Transactions on Neural Networks*, 9(6):1301–1318, 1998.

G.A. Tagliarini and E.W. Page. Solving constraint satisfaction problems with neural networks. In *The First IEEE International Conference on Neural Networks*, volume 3, pages 741–747. IEEE, 1987.