UNIFIED NEURAL REPRESENTATION MODEL FOR PHYSICAL AND CONCEPTUAL SPACES

ABSTRACT

The spatial processing system of the brain uses grid-like neural representations (grid cells) for supporting vector-based navigation. Experiments also suggest that neural representations for concepts (concept cells) exist in the human brain, and conceptual inference relies on navigation in conceptual spaces. We propose a unified model called "disentangled successor information (DSI)" that explains neural representations for both physical and conceptual spaces. DSI generates grid-like representations in a 2-dimensional space that highly resemble those observed in the brain. Moreover, the same model creates concept-specific representations from linguistic inputs, corresponding to concept cells. Mathematically, DSI vectors approximate value functions for navigation and word vectors obtained by word embedding methods, thus enabling both spatial navigation and conceptual inference based on vector-based calculation. Our results suggest that a single principle can explain computation of physical and conceptual spaces in the human brain.

1 INTRODUCTION

In the brain, grid cells in the entorhinal cortex (EC) represent the space by grid-like representations (Hafting et al., 2005; Doeller et al., 2010; Jacobs et al., 2013). This neural representation is often related to vector-based spatial navigation because grid cells provide global metric over the space. Theoretically, an animal can estimate the direction to a goal when representations of a current position and a goal position are given (Fiete et al., 2008; Bush et al., 2015). Furthermore, self-position can be estimated by integrating self-motions when sensory information is not available (McNaughton et al., 2006). These functions are the basis of robust spatial navigation by animals.

On the other hand, there are not only spatial representations but also conceptual representations in EC. Neurons called as "concept cells" have been found in human medial temporal lobe including EC (Quiroga, 2012; Reber et al., 2019). Concept cells respond to specific concepts, namely, stimuli related to a specific person, a famous place, or a specific category like "foods" and "clothes". Furthermore, recent experiments also suggest that grid-like representations appear not only for physical space but also for conceptual space if there is a 2-dimensional structure (e.g. lengths of a neck and legs, intensity of two odors), and those representations are the basis of vector-based conceptual inference (Bao et al., 2019; Constantinescu et al., 2016; Park et al., 2021). Thus, it is expected that there is a shared processing mechanism for physical and conceptual spaces in EC. However, a principle behind such universal computation in the brain is still unclear.

In this paper, we propose a representation model which we call disentangled successor information (DSI) model. DSI is an extension of successor representation (SR), which stems from a theory of reinforcement learning and became one of promising computational models of the hippocampus and EC (Dayan, 1993; Stachenfeld et al., 2017; Momennejad et al., 2017; Momennejad, 2020). Like dimension-reduced SR, DSI forms grid-like codes in a 2-D space, and those representations support vector-based spatial navigation because DSI approximates value functions for navigation in the framework of linear reinforcement learning (Todorov, 2006; 2009; Piray & Daw, 2021). Furthermore, when we apply DSI to text data by regarding a sequence of words as a sequence of states, DSI forms concept-specific representations like concept cells, by which we can perform vector-based conceptual inference like word embedding models in natural language processing (NLP) (Mikolov et al., 2013a;b; Pennington et al., 2014; Levy & Goldberg, 2014). For example, by calculating DSI vectors as "king"-"man"+"woman", we obtain a vector for "queen". Our model reveals a new

theoretical relationship between spatial and conceptual representation learning, and suggests a hypothesis that compressed information of successor states learned in the hippocampus and EC is the basis of unified neural processing mechanism for physical and complex conceptual spaces.

2 RELATED WORKS

Our model is related to the theory of reinforcement learning, cortical functions for spatial navigation, and learning of semantic concepts. There are previous works about each of these three topics. However, our model newly establishes connections between these topics, and offers a theoretical basis of unified spatial representations for physical and conceptual spaces.

Our model is an extension of successor representation (SR), which is recently viewed as a plausible model of hippocampus and EC (Dayan, 1993; Stachenfeld et al., 2017; Momennejad et al., 2017; Momennejad, 2020). Furthermore, default representation (DR), which is based on the theory of linear reinforcement learning, has been also proposed as a model of EC (Piray & Daw, 2021). Our model can be also viewed as a model of EC, and there is a relationship between our model and linear reinforcement learning. However, we show the relationship betweeen our model and conceptual learning, which has not been shown for SR and DR. Furthermore, we show vector-based compositionality of semantic concepts in our model. This finding expands the range of compositionality of EC representations (Piray & Daw, 2021) to semantic processing.

As a model of EC, our model forms grid-like representations in a 2-D space and they support spatial navigation. Previous studies have revealed that compression of place-specific activity patterns (place cells) under non-negative constraints is a key to generate realistic grid-like representations (Dordek et al., 2016; Sorscher et al., 2019). Furthermore, it was recently shown that a neural network model can learn grid-like representations from visual and motor signals, and those representations support efficient spatial navigation (Banino et al., 2018). Our model also depends on non-negativity to produce biologically plausible representations, and enables spatial navigation based on grid-like representations. However, previous models did not fully clarify theoretical properties of grid-like representations, especially mathematical relationships with reinforcement learning and word embedding methods. Our model deepens theoretical interpretations of grid-like representations and extends the range of application to general decision making and conceptual processing.

Vector-based analogical inference by our model is a same function as word embedding methods in NLP (Mikolov et al., 2013a;b; Pennington et al., 2014; Levy & Goldberg, 2014). However, a unique feature of DSI representation vectors is that each dimension of vectors corresponds to a specific concept like concept cells in the human brain (Quiroga, 2012; Reber et al., 2019), and each word is represented by a combination of concepts. Furthermore, previous word embedding methods have been developed only for NLP, thus relationships with other functions such as reinforcement learning and spatial navigation have not been extensively explored. It was recently shown that transformer-based models (Vaswani et al., 2017; Brown et al., 2020), which are currently state-of-the-art models in NLP, generate grid-like representations when those models are applied to spatial learning (Whittington et al., 2022). Similarly to our model, this finding implies the relationship between spatial and linguistic processing in the brain. However, the emergence of concept-specific representations and clear theoretical interpretability are still unique features of our model.

3 MODEL

3.1 SUCCESSOR REPRESENTATION

Let us assume N_s discrete states exist in the environment. Successor representation (SR) between two states s and s' is defined as

$$SR(s, s') = E\left[\sum_{t=0}^{\infty} \gamma^t \delta(s_t, s') | s_0 = s\right] = \sum_{t=0}^{\infty} \gamma^t P(s_t = s' | s_0 = s), \qquad (1)$$

where $\delta(i, j)$ is Kronecker's delta and γ is a discount factor.

SR is a variant of value functions in reinforcement learning, thus we can use various methods such as temporal-difference (TD) learning for the construction. Throughout this study, we used

a direct count method because we performed only offline processing of finite data. In a sequence of states $\{s_1, \ldots, s_t, \ldots, s_T\}$, we recursively calculated exponential traces of past states $z(s,t) = \sum_{\tau=0}^{t-1} \gamma^\tau \delta(s_{t-\tau}, s)$ as

$$z(s,t) = \gamma z(s, t-1) + \delta(s_t, s), \tag{2}$$

and calculated SR from state counts and coincidence counts as

$$SR(s, s') = \frac{\sum_{t=1}^{T} z(s,t)\delta(s_t, s')}{\sum_{t=1}^{T} \delta(s_t, s)}. \tag{3}$$

3.2 DISENTANGLED SUCCESSOR INFORMATION

Based on SR, we define successor information (SI) and positive successor information (PSI) as

$$SI(s, s') = \log(SR(s, s')) - \log(P(s')), \tag{4}$$

$$PSI(s, s') = \max\{SI(s, s'), 0\}. \tag{5}$$

In this study, we regard this quantity as a hippocampal model instead of SR (Figure 1A).

Next, we introduce a novel dimension reduction method which we call decorrelative non-negative matrix factorization (decorrelative NMF). Decorrelative NMF can be regarded as a variant of NMF (Lee & Seung, 1999) with additional constraints of decorrelation. By applying decorrelatve NMF to PSI, we obtain representation vectors called as disentangled successor information (DSI), which we regard as a model of EC (Figure 1A). In decorrelative NMF, we obtain D-dimensional vectors $\boldsymbol{x}(s)$ and $\boldsymbol{w}(s)$ ($D < N_s$) by minimization of the following objective function

$$J = \frac{1}{2} \sum_{s,s'} \rho(s, s')(PSI(s, s') - \boldsymbol{x}(s) \cdot \boldsymbol{w}(s'))^2$$

$$+ \frac{1}{2}\beta_{cor} \sum_{i \neq j} (Corr(i,j))^2 + \frac{1}{2}\beta_{reg} \sum_s (||\boldsymbol{x}(s)||^2 + ||\boldsymbol{w}(s)||^2), \tag{6}$$

subject to non-negative constraints $\forall i, x_i(s) \geq 0, w_i(s) \geq 0$. $\rho(s, s')$ is a weight for the square error

$$\rho(s, s') = \frac{1}{N_s V}\left(\frac{1}{M}PSI(s, s') + \rho_{min}\right), \tag{7}$$

where M and V are mean and variance of PSI, respectively, and ρ_{min} is a small value to avoid zero-weight. $Corr(i,j)$ is a correlation between two dimensions in $\boldsymbol{x}(s)$

$$Corr(i,j) = \frac{\sum_s \tilde{x}_i(s)\tilde{x}_j(s)}{\sqrt{\sum_s (\tilde{x}_i(s))^2 \sum_s (\tilde{x}_j(s))^2}}, \tag{8}$$

where $\tilde{x}_i(s) = x_i(s) - \frac{1}{N_s}\sum_s x_i(s)$. The first term of the objective function is weighted approximation error minimization, the second term works for decorrelation between dimensions, and the third term regularizes representation vectors. Optimization was performed by Nesterov's accelerated gradient descent method (Nesterov, 1983) with rectification of $x_i(s), w_i(s)$ every iteration. We describe additional details in Appendix A.1.

Figure 1: Interpretation of our model. (A) Biological interpretation of our model. PSI as a model of the hippocampus and DSI as a model of EC. (B) The setting of a state transition map in which DSI approximates value functions for spatial navigation.

3.3 MATHEMATICAL RELATIONSHIP WITH REINFORCEMENT LEARNING THEORY

In this section, we show that our model approximates value functions of linear reinforcement learning (Todorov, 2006; 2009; Piray & Daw, 2021) in the setting of spatial navigation.

In linear reinforcement learning, an agent aims to maximize "gain" instead of reward. Assuming a default policy $\pi^d(s)$ (any policy is available; typically random walk in the case of exploration task), gain function is defined as

$$g(s) = r(s) - \lambda KL(\pi(s)|\pi^d(s)), \tag{9}$$

where $r(s)$ is expected reward at the state s and $\lambda KL(\pi(s)|\pi^d(s))$ is the cost imposed on the difference between the current policy $\pi(s)$ and the default policy $\pi^d(s)$ (λ is a relative weight of the cost). Then, previous works have shown that the optimal policy and corresponding value functions can be determined explicitly by solving linear equations (Todorov, 2006; 2009; Piray & Daw, 2021). Here we consider an environment that consists of N_N non-terminal states and N_T terminal states. We define two transition probability matrices under the default policy: $\boldsymbol{P}_{NT}$ is a $N_N \times N_T$ matrix for transitions from non-terminal states to terminal states, and $\boldsymbol{P}_{NN}$ is a $N_N \times N_N$ matrix for transitions across non-terminal states. Furthermore, $\boldsymbol{r}_N$ and $\boldsymbol{r}_T$ are vectors of rewards at non-terminal states and terminal states, respectively. In this condition, a vector of value functions under optimal policy $\boldsymbol{v}^* = (v^*(s_1), \ldots, v^*(s_{N_N}))$ is obtained as

$$\exp(\lambda^{-1}\boldsymbol{v}^*) = \boldsymbol{M}\boldsymbol{P}_{NT}\exp(\lambda^{-1}\boldsymbol{r}_T), \tag{10}$$

where $\boldsymbol{M} = (\text{diag}(\exp(-\lambda^{-1}\boldsymbol{r}_N)) - \boldsymbol{P}_{NN})^{-1}$ is DR (Piray & Daw, 2021).

To relate $\boldsymbol{v}^*$ to SI, we consider a specific condition in which the environment consists of non-terminal states, and a virtual terminal state is attached to a goal state s_G arbitrarily chosen from non-terminal states (Figure 1B). When the agent gets to the goal, it transits to the terminal state with a probability p_{NT}. Furthermore, we assume that reward at non-terminal states are uniformly negative and reward at the terminal state is positive so that the agent has to take a short path to goal to maximize reward. Specifically, we assume all elements of $\boldsymbol{r}_N$ are $\lambda\log\gamma$, and $r_T = -\lambda(\log\gamma + \log p_{NT} + \log P^d(s_G))$ where γ is an arbitrary value in the range $(0, 1)$, and $P^d(s_G)$ is a probability of visiting the state s_G under the default policy. Then, we obtain

$$\exp(\lambda^{-1}\boldsymbol{v}^*) = \frac{1}{P^d(s_G)}(\boldsymbol{I} - \gamma P_{NN})^{-1}\boldsymbol{e}^{(i_G)}, \tag{11}$$

where $\boldsymbol{e}^{(i_G)} = (0, \ldots, 0, 1, 0, \ldots, 0)^T$ (i_G is the index of the goal state).

Because $(\boldsymbol{I} - \gamma P_{NN})^{-1}$ is equivalent to a successor representation matrix with a discount factor γ (Dayan, 1993; Stachenfeld et al., 2017), we finally obtain

$$\lambda^{-1}v^*(s) = \log(SR^d(s, s_G)) - \log P^d(s_G) = SI^d(s, s_G) \approx \boldsymbol{x}(s) \cdot \boldsymbol{w}(s_G), \tag{12}$$

where $SR^d(s, s_G)$ and $SI^d(s, s_G)$ are SR and SI under the default policy, respectively. Thus, SI is proportional to value functions for spatial navigation and inner products of DSI vectors approximates value functions. Based on this interpretation, we basically regard $\boldsymbol{x}(s)$ as a representation of each state, and $\boldsymbol{w}(s)$ represents a temporary goal.

3.4 MATHEMATICAL RELATIONSHIP WITH WORD EMBEDDING METHODS

On the other hand, DSI is related to word embedding methods in NLP (Mikolov et al., 2013a;b; Pennington et al., 2014; Levy & Goldberg, 2014). In linguistics, pointwise mutual information (PMI) and positive pointwise mutual information (PPMI) are used to measure the degree of coincidence between two words (Levy & Goldberg, 2014). They are defined as

$$PMI = \log\left(\frac{P(word_i, word_j)}{P(word_i)P(word_j)}\right), \tag{13}$$

$$PPMI = \max\{PMI, 0\}, \tag{14}$$

where $P(word_i, word_j)$ is a coincidence probability of two words (in a certain temporal window). It has been proven that dimension reduction of PMI approximates a famous word embedding method

skip-gram (Mikolov et al., 2013a;b) and similar performance can be obtained using PPMI (Levy & Goldberg, 2014). GloVe (Pennington et al., 2014) is also based on this perspective.

SI can be written as

$$SI(s, s') = \log(SR(s, s')) - \log(P(s')) = \log\left(\frac{\sum_{t=0}^{\infty} \gamma^t P(s_t = s', s_0 = s)}{P(s)P(s')}\right). \quad (15)$$

In this formulation, we can see mathematical similarity between PMI and SI, thus the correspondence between PPMI and PSI. Because of this relationship, we can expect that DSI, which is obtained through dimension reduction of PSI, has similar properties to word embedding methods. The difference is how to count coincidence: the coincidence in SI is evaluated with an asymmetric exponential kernel as in SR, in contrast that a symmetric rectangular temporal window is often used in typical word embedding.

Discussion above has shown dual interpretation of our model. On the one hand, DSI approximates value estimation of linear reinforcement learning, thus support goal-directed decision making and navigation. On the other hand, the same representation approximates word embedding in NLP, thus support semantic computation.

4 LEARNING REPRESENTATIONS OF PHYSICAL SPACES

In this section, we empirically show that DSI model forms biologically plausible grid-like representations in a 2-D physical space, and they support spatial navigation. These results also apply to conceptual spaces with the 2-D structure, depending on the definition of states.

4.1 LEARNING PROCEDURE

As an environment, we assumed a square room tiled with 30×30 discrete states (Figure 2A). In each simulation trial, an agent starts at one of those 900 states and transits to one of eight surrounding states each time except that transitions are limited at states along the boundary (the structure was not a torus). Transitions to all directions occur with an equal probability. We performed 500 simulation trials and obtained a sequence of 100,000 time steps in each trial. We calculated occurrence probabilities ($P(s)$) and a successor representation matrix ($SR(s, s')$) of 900 states from those sequences, and calculated PSI and DSI (100-dimensional) as described in the Model section. The discount factor γ was set to 0.99. We additionally tested spatial navigation in a structure with separated and interconnected rooms (see Figure 3C). In that case, we used the discount factor $\gamma = 0.999$.

4.2 EMERGENCE OF GRID-LIKE REPRESENTATIONS

Here we call each dimension of DSI representation vectors $\boldsymbol{x}(s)$ as a neural "unit", and we regard a value in each dimension at each state as a neural activity (or a neural representation). As shown in Figure 2B, many units exhibited grid-like activity patterns in the space. We performed a gridness analysis that has been used in previous animal experiments (Sargolini et al., 2006) and found that 51% of units were classified as grid cells.

Furthermore, we checked whether DSI representations in the physical space reproduce a property of biological grid cells. Actual grid cells in the rat brain exhibit multiple discrete spatial scales and the ratio between grid scales of adjacent modules is $\sqrt{2}$ (Stensola et al., 2012). We constructed a distribution of grid scales of DSI units by kernel density estimation, which revealed that multiple peaks of grid scales existed and the ratio between grid scales of adjacent peaks was $\sqrt{2}$ (Figure 2C). These results show that DSI model constructs biologically plausible grid-like representations in the 2-D physical space. We describe details of analysis methods in Appendix A.2.

4.3 NEAR-OPTIMAL SPATIAL NAVIGATION BY DSI VECTORS

As discussed in Section 3.3, the inner product of DSI representations approximate value functions for spatial navigation. Therefore, we tested whether DSI representations actually enable near-optimal navigation in the space.

Figure 2: DSI representations for the physical space. (A) The square room tiled with 30x30 discrete states. (B) Grid-like DSI representations in the space (upper) and their spatial autocorrelation (lower). (C) The distribution of grid scales of DSI representations. Red and blue broken lines indicate positions of peaks and $\frac{30}{(\sqrt{2})^n}$, respectively.

Figure 3: Spatial navigation using DSI representation vectors. (A) Geometric interpretation of the state transition rule in the DSI representation space. (B) An example spatial path obtained by DSI-based navigation. (C) Example spatial paths by DSI-based navigation in the four-room environment.

We assume that a start location (state s_{init}) and a goal location (state s_G) are randomly given in each trial such that the shortest path length is minimally 10, and an agent has to navigate between them. To solve the task, we define a vector-based state transition rule. Suppose that the agent exists at a state s, and a set of neighboring states of s is $\mathbb{A}(s)$. Given the goal representation vector $\boldsymbol{w}(s_G)$, a value function of a neighboring state $s_{next} \in \mathbb{A}(s)$ is estimated by $\boldsymbol{x}(s_{next}) \cdot \boldsymbol{w}(s_G)$, and the agents transits to the state that has a maximum value. This state transition rule can be geometrically interpreted as the choice of movements that has the closest angle with the goal vector in the representation space (Figure 3A). Otherwise, we can interpret that the agent estimates value functions by linear readout from grid-like DSI representations. Because of the approximation error, this rule did not always give optimal navigation (the shortest path from the start to the goal). However, the agent could take the shortest path to the goal in 93.9% of 1,000 trials we tested (an example is shown in Figure 3B). Furthermore, 97.2% were near-optimal navigation in which the actual path length was shorter than 1.1 times the shortest path length. The same framework also worked in a relatively complex environment with separated rooms (Figure 3C). In this environment, the ratio of optimal and near-optimal navigation was 68% and 82.6%, respectively. These results shows that DSI representations can support spatial navigation, which corresponds to the contribution of biological grid cells for spatial navigation (McNaughton et al., 2006; Fiete et al., 2008; Bush et al., 2015).

Figure 4: Vector-based inference of a novel spatial context. (A) We constructed representation vectors for a novel context A+B (a square room with two barriers) by the sum of DSI representation vectors for two familiar contexts A and B (with either of two barriers). (B) Rates of near-optimal navigation in various settings of representation vectors and contexts.

4.4 VECTOR-BASED INFERENCE OF SPATIAL CONTEXTS

We additionally found that we can perform vector-based inference for spatial navigation in a novel context. First, we constructed DSI representation vectors in spatial contexts A and B, each of which has a barrier (Figure 4A). Then, we created representation vectors for a novel context A+B with two barriers by simply adding representation vectors for familiar contexts A and B (Figure 4A). We tested vector-based navigation (described in the section 4.3) in three spatial contexts A, B, and A+B, using one of three representations for A, B, and A+B. Naturally, representation vectors for A and B gave the best performance in contexts A and B, respectively (Figure 4B). Notably, composite representation vectors for A+B achieved the best performance in the context A+B (Figure 4B). This result suggests that we can utilize vector-based composition of representations for a novel spatial context. We describe details of the simulation in Appendix A.3.

5 LEARNING REPRESENTATIONS OF CONCEPTUAL SPACES

In this section, we show that the same DSI model can learn representations for a complex conceptual space from linguistic inputs, and those representations support vector-based conceptual inference.

5.1 LEARNING PROCEDURE

We used text data taken from English Wikipedia, which contains 124M tokens and 9376 words (see Appendix A.4 for the detail of preprocessing). To construct DSI representations, we regarded each word as a "state", and considered the text data as a sequence of 9376 states ($N_s = 9376$). Then, we applied the exactly same learning procedure as in the experiment of physical spaces. We obtained 300-dimensional DSI representation vectors for each word. The discount factor γ was set to 0.9. The setting of other parameters was the same as the experiment of physical spaces.

5.2 EMERGENCE OF CONCEPT-SPECIFIC REPRESENTATIONS

As in the previous section, we regard each dimension of representation vectors as a neural unit, and checked how various words activate those units. Specifically, we listed ten words that elicited the highest activities in each unit (TOP-10 words). Consequently, we found that many units are activated by words related to specific concepts (Figure 5; other examples in Appendix A.8), which could be named as "game cell" or "president cell", for example. We quantified this conceptual specificity through WordNet-based semantic similarity between words (Princeton University, 2010). We compared mean similarity among TOP-10 words and a null distribution of similarity between random word pairs, by which we determined statistically significant concept-specific units and quantified the degree of conceptual specificity of each unit (see Appendix A.5 for details). DSI exhibited the larger number of significantly concept-specific units and higher average conceptual specificity than other well-established word embedding methods such as skip-gram and GloVe (Table 1) (Mikolov et al., 2013a;b; Pennington et al., 2014; Levy & Goldberg, 2014). This result shows that, unlike typical word embedding methods, our DSI model forms better concept-specific representations. However, we unexpectedly found that continuous-bag-of-words (CBOW) showed high conceptual specificity. Further investigation may be necessary to reveal the relationship between CBOW and DSI.

TOP 10 words for each unit

Unit 9	Unit 31	Unit 113	Unit 244	Unit 269
eleventh 2.13	orbit 2.16	playstation 2.38	covid-19 1.84	reagan 1.84
tenth 2.09	spacecraft 2.12	nintendo 2.25	virus 1.76	obama 1.81
ninth 2.00	saturn 1.95	xbox 2.13	infected 1.71	barack 1.78
seventh 1.96	apollo 1.84	console 1.93	pandemic 1.65	bush 1.61
eighth 1.95	lunar 1.80	arcade 1.78	viral 1.64	trump 1.55
twelfth 1.95	planets 1.78	360 1.62	epidemic 1.62	clinton 1.53
7th 1.93	nasa 1.73	gameplay 1.56	hiv 1.50	presidents 1.35
8th 1.86	mars 1.73	pc 1.46	plague 1.42	roosevelt 1.31
10th 1.84	moon 1.69	mario 1.40	infections 1.39	nixon 1.30
11th 1.84	orbital 1.66	metacritic 1.33	outbreak 1.37	presidential 1.29
Order cell	*Space cell*	*Game cell*	*Virus cell*	*President cell*

Figure 5: Concept-specific representations formed by DSI. Ten words that gave the highest activation (TOP-10 words) are shown. We also marked each unit with a descriptive label.

Table 1: Evaluation of conceptual specificity. Numbers of evaluated and significantly concept-specific units, the ratio of concept-specific units, and average conceptual specificity are summarized.

METHOD	EVALUATED	SIGNIFICANT	RATIO	SPECIFICITY
DSI	285	100	35%	0.32
Skip-gram	297	14	5%	-0.11
CBOW	298	83	28%	0.26
GloVe	297	6	2%	-0.07
PPMI-SVD	297	36	12%	0.06

5.3 Vector-based computation in the conceptual space

Given that DSI and word embedding methods are mathematically similar (Section 3.4), we expect that DSI representation vectors have similar properties to representation vectors learned by those word embedding methods. We evaluated the performance of DSI representation vectors in two tasks that have been used to evaluate word embedding methods: word similarity and analogical inference (Mikolov et al., 2013a;b; Pennington et al., 2014; Levy & Goldberg, 2014). In the word similarity task, we calculated cosine similarity between representation vectors of word pairs, and evaluated the rank correlation between those cosine similarities and human word similarities (WS353 dataset (Agirre et al., 2009); 248/345 word pairs were used). In the analogical inference task, we performed calculation of vectors such as $\boldsymbol{x}(king) - \boldsymbol{x}(man) + \boldsymbol{x}(woman)$ and checked whether the resultant vector has the maximum cosine similarity with $\boldsymbol{x}(queen)$ (Mikolov's dataset (Mikolov et al., 2013a;b); 3157/19544 questions were used; some examples in Appendix A.7). The result (Table 2) shows that DSI representation vectors achieved comparable performance with other well-established word embedding methods. Thus, similarity of DSI representation vectors corresponds to word similarity, and conceptual inference is possible through intuitive composition of DSI vectors like the inference of the novel spatial context in the section 4.4.

6 Discussion

In this paper, we proposed a theoretically interpretable and biologically plausible neural representation model for physical and conceptual spaces. We demonstrated that our DSI model forms grid-like representations in physical spaces and concept-specific representations in conceptual spaces, which are assumed to correspond to neural representations in EC. According to additional analyses (see Appendix A.6), decorrelative NMF is crucial for those representations. Furthermore, we showed that SI is mathematically related to linear reinforcement learning and word embedding methods, thus DSI representations supporting spatial navigation and conceptual inference. These results sug-

Table 2: Performances of vector-based computations in the conceptual space. The correlation of word similarity evaluated by vectors and humans, and the rate of correct analogical inference.

METHOD	SIMILARITY	ANALOGY
DSI	0.70	0.63
Skip-gram	0.69	0.71
CBOW	0.69	0.74
GloVe	0.69	0.71
PPMI-SVD	0.52	0.58

gest that spatial and conceptual processing can be theoretically unified into a single vector-based computational principle, and the spatial processing system in the brain may rely on that principle.

In contrast with successor representation which is tightly related to value functions in conventional reinforcement learning, our DSI model approximates value functions in linear reinforcement learning. An important feature of linear reinforcement learning is that value functions are directly determined from representations learned under a default policy, while rigorous calculation of conventional value functions requires representations under an optimal policy. It would be intriguing to clarify the relationship between a choice of default policy and the bias of representations and navigation functions (Piray & Daw, 2021), which may correspond to the experimentally observed distortion of grid cells (Boccara et al., 2019). Furthermore, how we can extend such theoretical concepts of reinforcement learning into conceptual processing remains to be addressed. Such extension may open the way to understand conceptual processing from the theory of decision making.

In the section 5.2, we showed that our DSI model creates concept-specific representations from text data. To the best of our knowledge, such property has not been reported in any previous word embedding methods. However, in the field of deep generative models, "disentanglement" of latent representations enables the formation of visual feature-specific representations (Higgins et al., 2017). We speculate that our model performs something similar to such methods, that is, disentanglement of word representations. As disentangled visual representations explain neural activities in higher-order visual cortex (Higgins et al., 2021), we may similarly interpret concept cells in the human medial temporal lobe as disentangled conceptual representations. Furthermore, grid cells may also emerge as disentangled spatial representations for 2-D structures.

Our model implies the relationship between word embedding methods and conceptual representations in the brain. Previously, it was shown that word representation vectors obtained by Skip-gram support high-performance decoding of semantic information from the brain (Nishida & Nishimoto, 2018), which experimentally supports this idea. However, with regard to a biologically plausible linguistic representation model, recent studies have shown that representations in transformer-based models (Vaswani et al., 2017) such as GPT (Brown et al., 2020) achieve great performance in linear fitting to neural recording (Goldstein et al., 2022; Schrimpf et al., 2021). A major difference between our DSI model and transformer-based models is that DSI representations are basically fixed (static embedding) whereas transformer-based models flexibly create context-dependent representations (dynamic embedding). Conceptual interpretation obviously depends on the context, thus activities of concept cells are context-dependent (Bausch et al., 2021). Therefore, our DSI model should be extended to process context-dependence, hopefully by combination with other models that enable learning of latent cognitive states (Uria et al., 2020; George et al., 2021; Whittington et al., 2020; 2022). This extension also leads to flexible decision making and navigation.

Another direction of future research is learning DSI representations from low-level sensory inputs, like spatial learning from visual and auditory inputs in previous models (Banino et al., 2018; Taniguchi et al., 2018; Uria et al., 2020). As for the human brain, infants probably form primitive spatial and conceptual representations from sensory signals, and later linguistic inputs enrich those representations. We speculate that real-world sensory data also contain the information of the conceptual space, for which DSI can be extended to learn those structures. Such model would clarify the role of the hippocampal system not only in spatial learning but also in conceptual learning.

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A APPENDIX

A.1 DETAILS OF DECORRELATIVE NMF

In decorrelative NMF, we iteratively updated vectors $\boldsymbol{x}(s)$ and $\boldsymbol{w}(s)$ by Nesterov's accelerated gradient descent method to minimize the objective function (Eq. 6), rectifying all elements every iteration. Gradients are

$$\frac{\partial J}{\partial x_k(s)} = -\sum_{s'} \rho(s, s')(PSI(s, s') - \boldsymbol{x}(s) \cdot \boldsymbol{w}(s'))w_k(s')$$

$$+ \beta_{cor} \sum_{j \neq k} \frac{Corr(k, j)\tilde{x}_j(s)}{\sqrt{\sum_s (\tilde{x}_k(s))^2 \sum_s (\tilde{x}_j(s))^2}} + \beta_{reg} x_k(s), \tag{16}$$

$$\frac{\partial J}{\partial w_k(s')} = -\sum_s PSI(s, s')(PSI(s, s') - \boldsymbol{x}(s) \cdot \boldsymbol{w}(s'))x_k(s) + \beta_{reg} w_k(s'). \tag{17}$$

We note that we regarded mean and variance of $x_i(s)$ in the correlation ($\frac{1}{N_s}\sum_s x_i(s), \sum_s (\tilde{x}_i(s))^2$ in Eq. 8) as constants in the calculation of these gradients. Practically, this heuristic did not affect the performance of decorrelation.

Throughout this paper, the learning rate was 0.05 and the number of iteration was 10000. Parameters were $\beta_{cor} = 1, \beta_{reg} = 0.001$, and $\rho_{min} = 0.001$.

A.2 DETAILS OF EVALUATION OF GRID REPRESENTATIONS

In the section 4.2, we performed the gridness analysis following a previous experimental study (Sargolini et al., 2006). For each unit, we rotated the spatial autocorrelation map (Figure 2B, lower) and calculated correlations between the original and rotated maps. Gridness was defined as the difference between the lowest correlation at $60°$ and $120°$ and the highest correlation at $30°$, $90°$ and $150°$. A unit was classified as a grid cell when gridness exceeds zero.

In Figure 2C, we constructed a distribution of grid scales. Grid scales were determined as the median of distances between the central peak and the six closest peaks (vertices of inner hexagon) in the spatial autocorrelation map. The kernel function for kernel density estimation was Gaussian with a standard deviation 1.

A.3 DETAILS OF VECTOR-BASED INFERENCE OF THE SPATIAL CONTEXT

In the section 4.4, we performed vector-based inference for spatial navigation in a novel context. Specifically, we define separated states in contexts A, B, A+B as s_i^A, s_i^B and s_i^{A+B}, where i is a positional index which indicates a same position in all contexts ($i = 1, 2, \cdots, 900$). We constructed representation vectors $\boldsymbol{x}(s_i^A)$, $\boldsymbol{w}(s_i^A)$, $\boldsymbol{x}(s_i^B)$, and $\boldsymbol{w}(s_i^B)$ through direct experiences, then we created $\boldsymbol{x}(s_i^{A+B})$ and $\boldsymbol{w}(s_i^{A+B})$ as

$$\boldsymbol{x}(s_i^{A+B}) = \boldsymbol{x}(s_i^A) + \boldsymbol{x}(s_i^B), \tag{18}$$

$$\boldsymbol{w}(s_i^{A+B}) = \boldsymbol{w}(s_i^A) + \boldsymbol{w}(s_i^B). \tag{19}$$

We performed spatial navigation in a given context using one of three representations $\{\boldsymbol{x}(s_i^A), \boldsymbol{w}(s_i^A)\}$, $\{\boldsymbol{x}(s_i^B), \boldsymbol{w}(s_i^B)\}$, and $\{\boldsymbol{x}(s_i^{A+B}), \boldsymbol{w}(s_i^{A+B})\}$ for corresponding positions, following the rule described in the section 4.3. In figure 6, we show structures of state transition graphs for three contexts A, B, and A+B.

To learn representations in contexts A and B, we sampled sequences of $\{s_i^A\}_{i=1,\cdots,900}$ and $\{s_i^B\}_{i=1,\cdots,900}$ by random walk in context A and B. The procedure was basically same with the section 4 except that we increased the number of simulation trials from 500 to 1,000, and state transition to the same position in the other context occurred every 5,000 time steps (transition between s_i^A and s_i^B). We added this transition to associate the same position in different contexts. It means that we assumed that the setting of barriers can change during the experience but this temporal association may be substituted by similarity of sensory inputs across contexts. From sampled sequences, we calculated PSI for all combinations of $\{s_i^A\}_{i=1,\cdots,900}$ and $\{s_i^B\}_{i=1,\cdots,900}$, and calculated 100-dimensional DSI vectors for 1,800 states by simultaneous compression of all states. The discount factor γ was set to 0.999.

Figure 6: Structures of state transition graphs used in the section 4.4.

A.4 DETAILS OF PREPROCESSING OF TEXT DATA

In the section 5, we used text data taken from English Wikipedia dump (enwiki-latest-pages-articles, 22-May-2020). We first generated text files from raw data using wikiextrator (`https://github.com/attardi/wikiextractor`). We tokenized texts by nltk Punkt sentense tokenizer, and randomly sampled 100,000 articles containing 1,000 tokens at minimum. We lowercased all characters and removed punctuation characters in the data. After that, we selected words that appeared more than 1,000 times in the data, and substituted all other rare words by <unk> symbol. Finally, we obtained data that contains 124M tokens and 9376 words.

A.5 DETAILS OF EVALUATION OF CONCEPTUAL SPECIFICITY

In the section 5.2, conceptual specificity of each unit was evaluated using WordNet database (Princeton University, 2010). In WordNet, a word belongs to several synsets (sets of cognitive synonyms), and semantic similarity of two synsets can be evaluated from the shortest path length between them in the WordNet structure (we used path_similarity function in nltk library). We defined similarity of two words as the highest similarity among all combinations of synsets of those words. We calculated mean similarity of all combinations of TOP-10 words (ten words that highly activated the unit; Figure 5A) that are available in WordNet. We evaluated only units which had at least five TOP-10 words available in WordNet. Furthermore, we randomly generated 1,000 pairs of words available in WordNet, and generated a null distribution of similarity between words. We defined a significance threshold of similarity as a 95 percentile of the null distribution, and a unit was classified as a significantly concept-specific unit if mean similarity of TOP-10 words exceeded the threshold. Furthermore, we quantitatively defined a conceptual specificity of each unit as

$$\frac{s_{unit}}{s_{null}} - 1, \tag{20}$$

where s_{unit} is mean similarity of TOP-10 words and s_{null} is the mean of the null distribution. This quantity becomes zero if similarity between TOP-10 words is not different from random pairs,

and becomes positive if TOP-10 words are semantically similar. This conceptual specificity was averaged over all evaluated units.

A.6 RELATIONSHIP BETWEEN MODEL COMPONENTS AND REPRESENTATIONS

To clarify the contribution of each model component to the results in this study, we performed a "lesion study" in which we removed some components in DSI and repeated the same evaluation procedure in the main text. We summarize results in Table 3. First, we tested representations obtained by singular value decomposition of successor representation (SR-SVD), which was regarded as a model of grid cells in a previous study (Stachenfeld et al., 2017). DSI model exceeded SR-SVD in all aspects shown in this study. Next, we tested DSI model without decorrelation ($\beta_{cor} = 0$) and DSI model without non-negativity (no rectification of representation vectors). Neither modification impaired the performance of navigation and inference, showing the importance of using SI for vector-based computations as theoretically expected. In contrast, removing decorrelation and non-negativity significantly impaired the emergence of grid-like units and concept-specific units, respectively. Thus, decorrelative NMF is crucial to obtain biologically plausible representations.

Table 3: Contribution of each model component to the performance. Rates of grid-like units, near-optimal navigation, significantly concept-specific units, correct analogical inference.

METHOD	GRID CELL	NAVIGATION	CONCEPT CELL	ANALOGY
Full DSI	51%	97.2%	35%	63%
Decorrelation OFF	5%	99.9%	38%	64%
Non-negativity OFF	29%	99.8%	2%	63%
SR-SVD	21%	57.2%	13%	28%

A.7 EXAMPLES OF THE ANALOGICAL INFERENCE TASK

In table 4, we show some examples of the analogical inference in Mikolov's dataset. There is a relationship "WORD1 is to WORD2 as WORD3 is to WORD4". Then, an expected relationship in the vector space is WORD2-WORD1=WORD4-WORD3. In this study, we performed inference of WORD4 by WORD3+WORD2-WORD1. We regarded an inference was correct if the actual vector of WORD4 had the largest cosine similarity to the inferred vector among all word representation vectors (except those for WORD1, WORD2, and WORD3). If the number of words is 10,000, a chance level of the correct answer rate is 0.01%. Therefore, the performance shown in this study (more than 50%) is far above the chance level.

Table 4: Examples of analogical relationships in Mikolov's dataset.

WORD1	WORD2	WORD3	WORD4
boy	girl	king	queen
husband	wife	he	she
Paris	France	Tokyo	Japan
China	Chinese	Italy	Italian
big	bigger	small	smaller
free	freely	quick	quickly
convenient	inconvenient	possible	impossible

A.8 EXAMPLE DSI REPRESENTATIONS FOR WORDS

In the figure 7, we show TOP-10 words of DSI units without manual selection. We found several non-significant units exhibit conceptual specificity according to manual inspection (for example, unit4 may be named as university cell). This is probably because of the limitation of knowledge covered by WordNet. Therefore, we suppose that the current evaluation method tends to underestimate the number of concept-specific units. However, the comparison across models was fair because we used the same procedure and criteria for all models.

Unit 1	Unit 2	Unit 3	Unit 4	Unit 5
faced	transit	humid	universities	sheets
overcome	commuter	winters	colleges	olivia
facing	trains	summers	uc	compact
due	bus	climate	usc	senators
owing	buses	mild	consortium	antony
citing	subway	precipitation	institutes	proposes
experiencing	rail	warm	carnegie	atlas
cope	passenger	temperatures	affiliated	spaces
amid	metro	cool	alumni	geometry
suffered	passengers	cold	selective	rough

Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
designers	rebounds	nbc	eleventh	nhl
scientists	assists	aired	tenth	confirmation
experts	averaged	abc	ninth	hockey
professionals	steals	airing	seventh	maple
consumers	nba	cbs	eighth	roller
researchers	averaging	syndicated	twelfth	judiciary
filmmakers	partition	programming	7th	flames
lawyers	points	broadcast	8th	devils
composers	prussia	channel	10th	batch
scholars	mvp	espn	11th	senators

Unit 11	Unit 12	Unit 13	Unit 14	Unit 15
lowest	valve	archive	hatch	rotten
ranked	wheel	archives	deaf	tomatoes
highest	steering	manuscripts	robot	metacritic
ranks	rotating	collections	suffrage	aggregate
literacy	wheels	collection	egg	approval
demographic	cylinder	manuscript	seymour	reviews
rising	trigger	library	salem	grossed
prevalence	shaft	catalogue	wwe	rating
ratings	pump	valuable	monte	byron
rank	gear	documents	resist	apparatus

Figure 7: A part of word representations formed by DSI. Ten words that gave the highest activation (TOP-10 words) are shown for units 1 - 15. Those classified as concept-specific units in our analysis are boxed with bold lines.