Generalizing to generalize: when (and when not) to be compositional in task structure learning

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Abstract

Humans routinely face novel environments in which they have to generalize in order to act adaptively. However, doing so involves the non-trivial challenge of deciding which aspects of a task domain to generalize. While it is sometimes appropriate to simply re-use a learned behavior, often adaptive generalization entails recombining distinct components of knowledge acquired across multiple contexts. Theoretical work has suggested a computational trade-off in which it can be more or less useful to learn and generalize aspects of task structure jointly or compositionally, depending on previous task statistics, but empirical studies are lacking. Here we develop a series of navigation tasks which manipulate the statistics of goal values ("what to do") and state transitions ("how to do it") across contexts, and assess whether human subjects generalize these task components separately or conjunctively. We find that human generalization is sensitive to the statistics of the previously experienced task domain, favoring compositional or conjunctive generalization when the task statistics are indicative of such structures, and a mixture of the two when they are more ambiguous. These results support the predictions of a normative "meta-generalization learning" agent that does not only generalize previous knowledge but also generalizes the statistical structure most likely to support generalization.

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It has long been proposed that rather than simply re-use past associations in a novel scenarios, humans can flexibly recombine components of prior knowledge to take novel actions (James, 1890). For example, an adept musician can learn multiple instruments by generalizing the motor skills needed to play across instruments, even as they use those skills for different effect across the different instruments. Conversely, they can transfer songs learned on one instrument to another even as the movements needed to play a song on the piano, for example, are very different than that of a guitar. In principle, the sequences of notes used to generate songs is distinct from of the skills needed to play an instrument: each is an independent component that can be combined with others arbitrarily. This degree of compositionality is critical for flexible goal-directed behavior but is often lacking in theoretical accounts of human and animal generalization.

Previous models have considered how agents and animals can cluster "latent states" across multiple contexts that share task statistics in both Pavlovian (Gershman, Blei, & Niv, 2010) and instrumental learning settings (Collins & Frank, 2013, 2016). These models assume each context acts as a pointer to a latent structure, and generalizing task statistics requires inference over which structure the current context belongs to. Similar principles have been employed in the machine learning literature for generalization by purely computational agents (Mahmud, Hawasly, Rosman, & Ramamoorthy, 2013; Rosman, Hawasly, & Ramamoorthy, 2016; A. Wilson, Fern, & Tadepalli, 2012). From a Bayesian perspective, this form of generalization falls under the domain of non-parametric clustering and relies on the Chinese Restaurant Process (CRP; Aldous, 1985) as a prior over clusters. The CRP is a popularity based process with no pre-determined number of clusters, but allows the number of clusters to grow with experience while favoring a smaller number of clusters. This form of clustering can be approximately implemented in corticostriatal neural networks endowed with hierarchical structure (Collins & Frank, 2013). These models have been used to explain

human generalization behavior and neural correlates thereof in a number of reinforcement learning tasks (Badre & Frank, 2012; Collins, 2017; Collins, Cavanagh, & Frank, 2014; Collins & Frank, 2013, 2016; Schulz, Franklin, & Gershman, 2018; Tomov, Dorfman, & Gershman, 2018).

However, the form of clustering assumed in these models, in which entire task structures are reused (or learned from scratch), can actually impede generalization in some cases (Franklin & Frank, 2018). In particular, the constituent knowledge within each task structure is inseparable: when some observations rule out a given task structure, the agent can no longer generalize any aspects of that structure, thereby preventing sharing of partial knowledge between contexts, requiring agents to relearn information they already have access to. While this type of data inefficiency is common in purely computational agents, humans share knowledge across contexts in a remarkably efficient manner (Lake, Ullman, Tenenbaum, & Gershman, 2016; Marcus, Marblestone, & Dean, 2014). This all-or-none generalization would, for example, prevent a musician from transferring a song learned on a piano to a guitar, given the differences in required motor actions to produce the desired notes. Furthermore, generalizing policies as a whole can be brittle, as policies and policy-dependent representations are often not robust to new tasks (Kansky et al., 2017; Lehnert, Tellex, & Littman, 2017).

Thus, given the evidentiary support of clustering models and the normative challenges posed by generalizing structures as a whole, one might expect clustering models to support component-wise generalization. This leads to the important question of how to choose a set of components to generalize. One natural choice from the perspective of reinforcement learning is to treat knowledge about state-transitions (the "transition function") as separate from knowledge about rewards (the "reward function"). This representation of structure is appealing because the two types of knowledge are independent and can be combined via planning to form a behavioral policy (Sutton & Barto, 1998).

Nonetheless, whether it is adaptive to independently generalize knowledge about

rewards and state-transitions is a statistical problem that varies with the properties of the task domain (Franklin & Frank, 2018). Generalizing these two components together is adaptive when knowledge of transitions is sufficiently informative about the rewards across contexts (i.e., they have mutual information), whereas generalizing each component independently adds a statistical bias to the inference of rewards that is adaptive when the relationship between components is weak, noisy, or difficult to discover. Consequently, a normative agent can maximize performance by inferring the overall statistical structure (independent or shared statistics between reward and transition functions) and arbitrating between the two forms of structure based on their accumulated evidence (Franklin & Frank, 2018). This meta-strategy suggests that the agent has access to both joint and compositional task representations and best makes use of them depending on the environment.

In the present work, we thus assessed whether human learning and generalization behavior could show evidence for compositionality, and further whether this behavior would depend on the extent to which external task statistics are suggestive of independent vs joint structures. We developed a series of navigation tasks in which subjects are able to learn goals ("where do you want to go?"; the reward function) independently from their learning which actions they need to take ("how can you get there?"; the transition function over states and actions). Both pieces of information are required to solve the task (i.e. to reach the reward). We varied the statistics of these two component features across contexts and tasks, such that the transition function was more or less informative about the reward function. We then assessed the degree to which humans were able to generalize these learned structures in novel contexts, and whether such generalization was consistent with joint (i.e., entire structure) or independent clustering. For each of the three tasks, we used computational modeling to generate qualitative predictions that differentiate between the independent or joint strategy (Franklin & Frank, 2018) and compared human subject performance to these *a priori* predictions.

Consistent with previous empirical studies on task structure learning, we found

subjects generalized learned knowledge in novel contexts across all three tasks, even as doing so was often costly (Collins, 2017; Collins & Frank, 2016). Critically, we find evidence that the degree of compositionality in generalization strategies depends on the previously encountered statistics of task structures, as predicted by the adaptive normative agent employing meta-generalization learning.

Results

Subjects completed a series of tasks in which they navigated a 6x6 grid-world on a computer in an attempt to discover the reward in one of a set of labeled goal locations across trials (Fig. 1). For simplicity, subjects learned a mapping between arbitrary keyboard presses and movements within the grid-world, as opposed to a complete state-action-state transition function[1]. Similar to the "finger sailing" task (A. Fermin, Yoshida, Ito, Yoshimoto, & Doya, 2010; A. S. Fermin et al., 2016), this design allows us to study subjects' ability to learn about mappings (state transitions) separately from the goal-values (reward function). Moreover, successful performance in the task requires model-based (i.e., goal-directed, rather than stimulus-response) control, which was ensured by varying the subjects' initial location and that of the goal from trial to trial, requiring flexible re-planning on each instance (Simon & Daw, 2011). Critically, many of the contexts share the same mapping and/or goal-values, and subjects can boost learning by leveraging this structure (Franklin & Frank, 2018).

To formally assess alternate learning and generalization strategies in the human navigation tasks, we adapted the computational models previously used to analyze the statistical tradeoff between compositional and joint structure learning (Franklin & Frank, 2018). These include a *joint clustering agent*, an *independent clustering agent* and a *meta-generalization agent* that dynamically arbitrates between the two (*Materials and Methods*). All three models are extensions of the joint clustering model proposed by

[1] Prior simulations in Franklin and Frank (2018) suggest that learning an action-movement mapping in leu of a full transition function does not influence the generalization tradeoffs discussed in the current work.

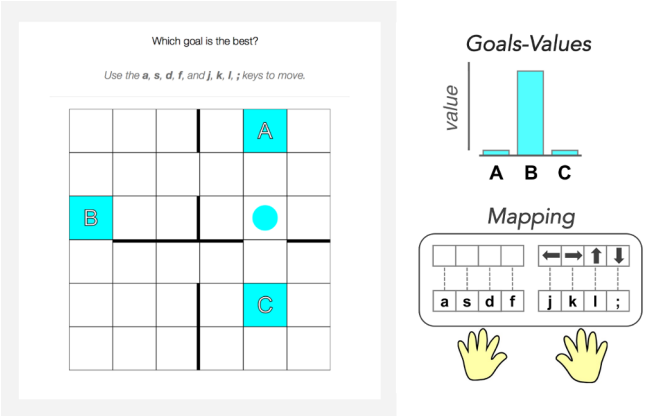

Figure 1. Subjects controlled a circle agent in a grid world (left) and navigate to one of three potential goals (colored squares labeled "A", "B", or "C"). Context was signaled to the subject with a shared color for the agent and goals. In each context, subjects learned the identity of the rewarded goal within the trial (top right) while also learning a mapping between the keyboard responses and the cardinal movement within the grid world (bottom right).

Collins and Frank (2013) to account for flexible re-use of learned structures across contexts, and make equivalent predictions on the types of instrumental stimulus-response tasks that have previously been investigated, wherein the reward values were not manipulated separately from the transitions (Collins et al., 2014; Collins & Frank, 2016). Each agent probabilistically assigning contexts into clusters that share similar observation statistics via Bayesian inference, with the observation statistics serving as the likelihood and the CRP as a context-popularity based prior. This allows the agents to reuse previously learned functions in novel contexts, and hence facilitating generalization. Moreover, these agents generalize task structure based on context popularity as a consequence of the CRP prior. In a new context, each agent will reuse task structure as a parametric function of how popular that task structure is across previously encountered contexts.

However, the agents differ by whether they cluster reward and transition functions as separate entities or jointly. The joint clustering agent clusters each context based on the "joint" (conjunctive) statistics of learned state transitions and reward functions (Fig

2). Such an agent, when attempting to generalize learned structures to new contexts, will use information it has gathered about the likely mappings to infer the likely goal values, but as such, it cannot reuse one independently of the other. This is equivalent to generalizing complete policies as indivisible structures. In contrast, the independent clustering agent clusters transitions and rewards separately by probabilistically assigning each context into two context-clusters, each associated with either a reward or transition function. Such an agent can make inferences about likely goal values that are not tied to any specific mapping, but as such, it cannot improve performance when the two functions are informative about each other. As neither fixed strategy is optimal across unknown task domains, the meta generalization agent dynamically arbitrates between joint and independent clustering based on the expected value of each[2], given the experienced task statistics in the environment.

In reinforcement learning problems, information about the transition structure is typically available prior to information about the reward value, and consequently the three agents differ largely in their generalization of reward functions (Franklin & Frank, 2018). While both agents generalize goal values as a function of their popularity across contexts, the joint clustering agent considers this popularity only for the subset of contexts that share the same mapping (in the musician example, this is like inferring what song to play based on its popularity conditioned on the set of instruments that share the same motor mappings). In contrast, the independent clustering agent generalizes goals by pooling across all contexts regardless of mappings. Thus, we can distinguish these model predictions by looking at goal generalization to see whether it varies as a function of mapping. Because the meta-agent arbitrates between these two strategies probabilistically, it predicts a dynamically weighted blend of the two across time.

We exploit this logic in the following grid-world tasks: in each task, subjects learn to navigate to reach a goal in a set of training contexts with varying overlap in

[2] The expected value of each strategy is approximately equivalent to the Bayesian model evidence for the strategy.

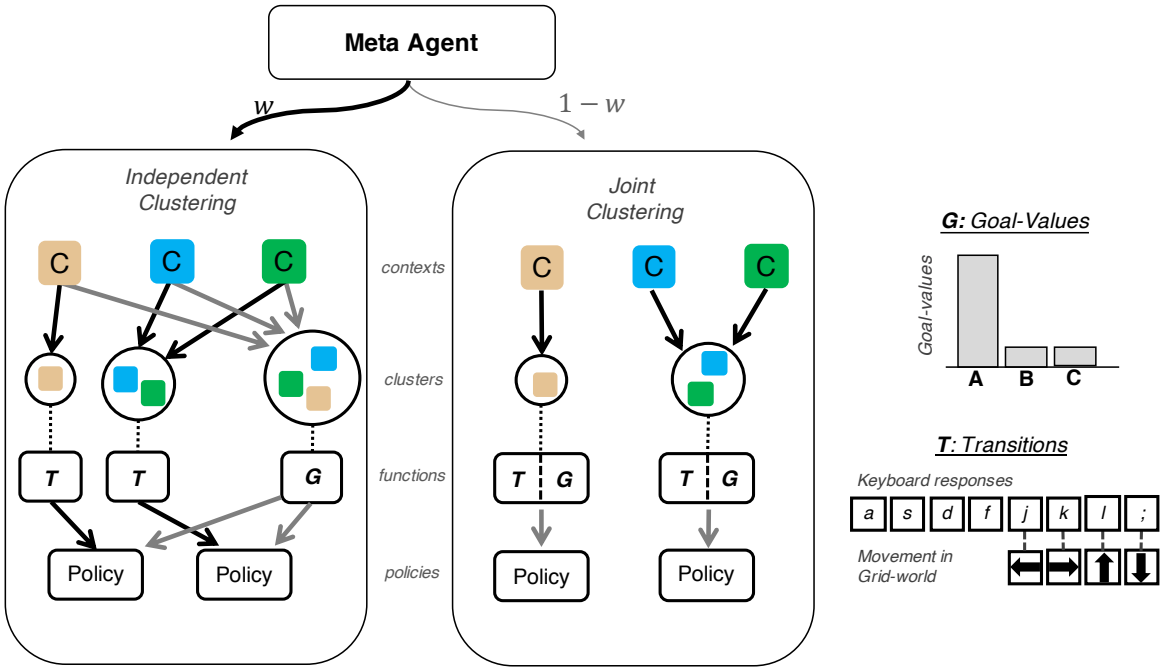

Figure 2. Schematic depiction of computational agent. The meta-generalization agent arbitrates between independent clustering and joint clustering according a learned weight w. In both clustering strategies, contexts (colored squares) are grouped into clusters based on the statistics of their associated goal (G) and transition (T) functions. Independent clustering clusters each context twice, once each for goal-value and transition functions, where as joint clustering assigns each context into a single cluster. Planning derives a behavioral policy from the learned contingencies. Adapted from (Franklin & Frank, 2018)

mappings and rewards, and are then probed for generalization in an unprompted set of novel contexts. Subjects are not told that it is possible to generalize (as it turns out in our designs, it is always advantageous to generalize mappings, but disadvantageous to generalize rewards in all but one of the experimental conditions). Critically, the degree to which mappings were informative of goal values was manipulated across experiments, allowing us to test whether subjects are sensitive to this structure. Across these three experiments, joint and independent clustering each predict a fixed and identifiable strategy, thus allowing us to qualitatively differentiate between the two on each task. The meta-agent, which predicts that subjects adaptively change their generalization

strategy to exploit the statistics of the task, varies in its behavior across the three tasks.

To preview the results, we find that subject generalization strategy changes with the task domain and is inconsistent with any single fixed generalization strategy. These results suggest that people rely on multiple strategies to generalize and adapt their behavior to be consistent with the statistics of their environment.

Experiment 1: Joint Structure

In the first experiment, subjects navigated grid-worlds in which there was a consistent relationship between the goal locations and the mappings, such that a given mapping was always paired with a given goal during training (Fig 3). This relationship is suggestive of joint structure and we hence tested whether subjects would later generalize this structure to novel contexts. Prior to an unsignalled generalization probe, subjects completed 32 trials across 3 training contexts, each of which was associated with one of two mappings and one of two potential goals. Subjects were instructed on the relationship between contexts, mappings and goals during a pre-training instruction but were not told how the relationships generalize between contexts. Subjects received binary reward (linked to financial payment) for selecting the correct goal and no reward for choosing the other goal. Two of the training contexts shared the same transitions and were paired with the same high popularity goal, while the third context was paired with the remaining goal and mapping. Thus, there was a one-to-one relationship between transitions and goals during training. To control for potential stimulus response biases, the number of trials within each context was balanced such that each each mapping and each correct goal was presented in the same number of trials (i.e., the context associated with the low popularity goal/mapping was presented twice as frequently as the other two contexts; Collins & Frank, 2016). In a subsequent test phase, subjects saw three novel contexts in which the joint statistics of the training contexts was either repeated (repeat condition) or switched (switch condition) in a between-subjects manipulation. However, the more popular goal in training (A) remained the more popular goal in testing, regardless of condition.

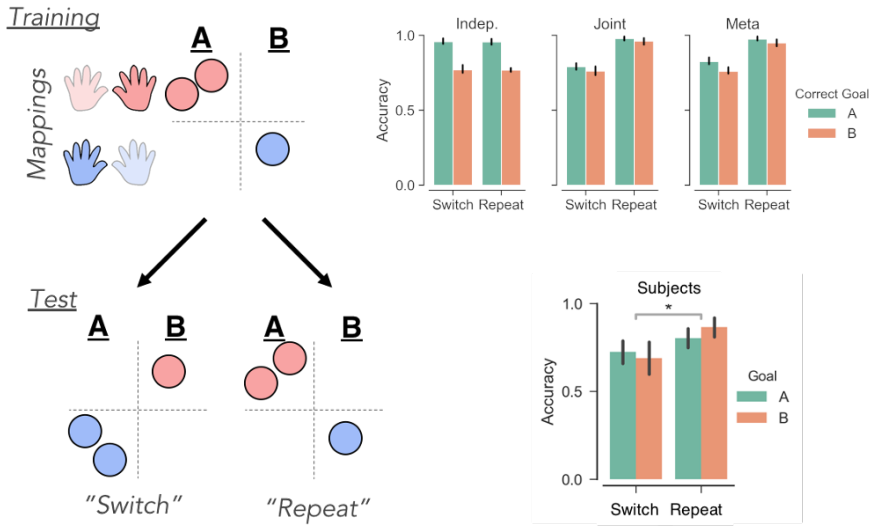

Figure 3. Experiment 1: Joint structure. *Left*: Task Design: During training, subjects saw three contexts (depicted here as circles) in which a given transition function (mappings, indicated by red/blue hands) was always paired with the same reward function (goals; A or B), suggestive of joint structure. In the test phase, subjects saw three novel contexts in which the relationship between transitions and goals was either repeated (i.e., each goal was paired with the same mapping as seen during training) or switched (goal B associated with the mapping that was previously paired with goal A). The switch vs. repeat manipulation was conducted between subjects. *Right, top row*: Model predictions as a function of test condition (switch vs repeat) and correct goal (green, orange). The joint clustering model leverages the relationships between goals and mappings and hence improves performance in the repeat condition. The independent clustering agent, in contrast, predicts better performance for the more popular goal A regardless of the switch vs repeat test condition. The meta agent shows a combination of the two but overall favors the pattern of the joint agent, given that the statistics during training are consistent with joint structure. *Right, bottom row*: Human subject behavior in the test contexts.

Computational modeling. We confirmed with our computational models (Franklin & Frank, 2018) that the independent and joint clustering agents are differentially sensitive to these manipulations. In particular, the joint clustering agent predicts better performance in the repeat condition (in which the goals are paired with the same mappings as during training, even in novel contexts) than in the switch condition (M=0.194, 95% highest posterior density interval (HPD) = [0.163, 0.231]), whereas the independent agent predicts no such effects (M=0.003, 95% HPD = [-0.027, 0.017]). Conversely, the independent agent predicts faster learning when the most popular goal is rewarded in either test context (Fig 3; M=0.189, 95% HPD = [0.161, 0.211]), whereas this effect is marginal in the joint agent (M=0.023, 95% HPD = [0.000, 0.059]). (Note that joint clustering *can* be sensitive to goal popularity for a given mapping; see experiment 2). Finally, the meta-generalization agent, which infers which structure is most likely during the training phase, is more similar to the joint agent (effect of test condition (M=0.168, 95% HPD = [0.133, 0.211])) but, like the independent agent, also shows a (much smaller) effect of the rewarded goal (M=0.05, 95% HPD = [0.009, 0.092]).

Human Behavior. The behavior of 129 subjects collected online via Amazon Mechanical Turk was carried through to analysis, 49 of which were randomly assigned the switch condition. During training, subject performance improved as a function of time as measured by rewards received, reaction time and navigation efficiency. Using Bayesian linear modeling, goal accuracy (rewards received) was found to increase as a function of trials within a context (Fig S3 A; $\mathbb{E}[\beta_t]$= 0.154, 95% HPD = [0.127, 0.182]) as was their speed (reciprocal reaction time) ($\mathbb{E}[\beta_t] = 0.048$: 95% HPD = [0.002, 0.098]). Navigation (in)efficiency, defined as the number of responses taken in excess of the minimum path length between the start location of the trial and the selected goal, also decreased as a function of trials within each context ($\mathbb{E}[\beta_t] = -0.012$, 95% HPD = [-0.015, -0.008]).

The primary measure of interest was goal accuracy in the test context, which differentiates the predictions of joint and independent clustering models (see above).

Goal accuracy was assessed with hierarchical Bayesian logistic regression that included test condition (switch vs repeat) as a between subjects measure and correct goal as a within subjects measure (see *Materials and Methods*). In addition, the number of trials experienced within the same context and whether a trial of the same context was sequentially repeated were included as nuisance regressors. Both nuisance regressors significantly predicted test accuracy (times in context: $\mathbb{E}[\beta_t] = 0.34$, 95% HPD=[0.223, 0.470]; sequential repeats: $\mathbb{E}[\beta_{\text{rep}}] = 1.623$, 95% HPD=[1.002, 2.214]). Consistent with the predictions of joint clustering and the meta-generalization agent, subjects were more accurate in the repeat condition than in the switch condition (Fig 3, $\mathbb{E}[\beta_{\text{switch}}] = -0.41$, 95%HPD = [-0.136, -0.151], $p_{\text{1-tail}} < 0.0005$). Accuracy did not vary as a function of the rewarded goal in the test contexts ($\mathbb{E}[\beta_{\text{goal}}] = 0.005$, 95% HPD = [-0.14, 0.15]).

Experiment 2: Independent Structure

While experiment 1 provided evidence for transfer of joint structure suggested as such by the training environment, this experiment alone does not suggest subjects would always generalize components jointly in all domains. Indeed, the meta-generalization agent (which combines independent and joint clustering and infers which is more likely) also showed behavior that was more similar to the joint agent. The behavior of the meta agent varies with the statistics of the task domain and thus can often produce similar behavior to a single, fixed strategy within a single experiment. Therefore, in experiment 2 we wished to test whether subjects would show evidence for independent, compositional, generalization when suggested to by the task environment. Because the meta-agent is sensitive to the conditional relationship between goals and mappings, we provided subjects with an environment where this relationship was very weak. Rather than the one-to-one relationship in experiment 1, the same goal could be re-used with different mappings, and the same mapping could be re-used with different goals, with some goals more popular than others (Fig 4 A). Subjects completed 112 trials in seven training contexts prior to a unsignaled generalization test with four novel contexts. Each training context was associated with one of two mappings and one

binary, deterministically rewarded goal location out of four possible locations.

Note that, as before, the independent clustering agent predicts that subjects learn about the statistics of goals and mappings independent of the other, and as such, they would learn about the popularity of goals across contexts regardless of mapping. For example, goal A is the most popular goal overall (marginalizing over mappings) but is equally popular as other goals within the contexts paired with the low popularity mapping (Fig 4 A, B; Table S2). Thus, independent and joint clustering make qualitatively different predictions about which goals will be searched first in a novel context as a function of the associated mapping. As such, subjects were given four novel contexts in an unsignaled test phase chosen to differentiate joint and independent clustering by crossing the *overall* goal popularity with the *conditional* goal popularity (conditioned on the mapping; Fig 4 A, B; Table S2). If subjects learn independent structure, then they should more rapidly learn for novel contexts associated with the more popular goal A (i.e., test context 1) even if it is paired with the low popularity mapping, whereas joint clustering predicts no such advantage. This same logic sets up three orthogonal within-subjects comparisons across the four test contexts that differentiate model predictions.

Computational Modeling. The computational models were simulated on the task to generate predictions in these contexts (see *Materials and Methods*). First, the key manipulation of interest is the difference in average reward between test context 1 and test context 2. The goals associated with the two test contexts have the same popularity during training, conditioned on the associated mapping (Fig. 4 A, B). However, because goal A is more popular overall, independent clustering predicts higher average reward in test context 1 relative to test context 2 (M=0.155, 95% HPD = [0.098, 0.216]), whereas joint clustering predicts no difference (M=-0.017, 95% HPD = [-0.077, 0.047]). Because the training environment is consistent with independent structure, the meta agent also predicts an advantage in context 1 (M=0.073, 95% HPD = [0.133, 0.133]).

Second, all three generalizing agents predict higher average reward in test contexts

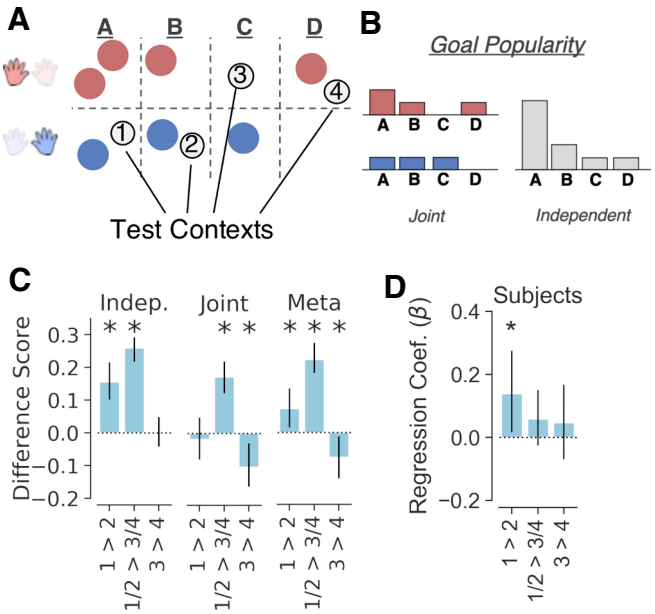

Figure 4. Experiment 2: Independent structure. *A*: Subjects saw six contexts (circles) during training, each paired with one of two mappings (*red*: high popularity, *blue*: low popularity) and one of four goals (A, B, C or D). Two of the high popularity goals were paired with multiple mappings, suggestive of independent structure. Subjects learned to navigate in an additional four novel test contexts following training (grey circles). *B*: Goal popularity in the training environment as a function of mapping (as tracked by a joint agent, left) and collapsed across all contexts (as tracked by an independent agent, right). *C*: Qualitative model predictions expressed as difference scores between test contexts for the independent clustering joint clustering and the meta-generalization agent . *D*: Regression weight of test context accuracy for subjects. Error bars reflect 95% HPD

1 and 2 than in test contexts 3 and 4, although this effect is slightly weaker for joint clustering (Fig. 4 C; independent: M=0.260, 95% HPD = [0.219, 0.2196]; joint M=0.172, 95% HPD = [0.126, 0.219]; meta agent: M=0.223, 95% HPD = [0.185, 0.273]). Third, given that test context 3 involves a goal that was never paired with the associated mapping during training, joint clustering predicts that test context 3 will be learned more slowly than test context 4 (M=-0.102, 95% HPD = [-0.161, -0.032]), whereas there was no such effect for independent clustering (M=0.002, 95% HPD = [-0.048, 0.058]). Because the training environment does not rule out some joint structure altogether (i.e., some goals are experienced multiple times with one mapping), the meta agent also predicts worse performance in context 3 than 4 (M=-0.075, 95% HPD = [-0.139, -0.013]). It is worth noting that, unlike the contrasts between test contexts 1 and 2, these two contrasts are largely driven by the parametric effects predicted by the CRP prior. While previous research has provided evidence that subjects generalize consistently with the CRP prior, this evidence was for the most popular structure and not evidence that subjects parametrically generalized task structure proportional to its relative popularity (Collins & Frank, 2016). That is, a non-zero value for these two contrasts is predicted largely by the difference in goal popularity between goals B, C and D, whereas a positive value of the contrast between test context 1 and 2 is driven by the difference in goal A (the most popular goal overall) and goal B.

Finally, and importantly, because of the nature of the test contexts chosen to differentiate the models, none of the generalizing agents achieved higher reward than a "flat" non-generalizing model that learns anew for each context (all p's $< 10^{-5}$ in favor of flat model over clustering agents in both training and test), suggesting the task design did not encourage subjects to generalize, even though other situations reveal substantial and compounding advantages for these generalization models (Franklin & Frank, 2018). Thus the test behavior in subjects indexes the degree to which they spontaneously generalize even when not incentivized by the task (Collins & Frank, 2013).

In addition to the average reward per context, the computational agents are further differentiated by the goals selected in the first trial of a new context (Fig. 5 A,

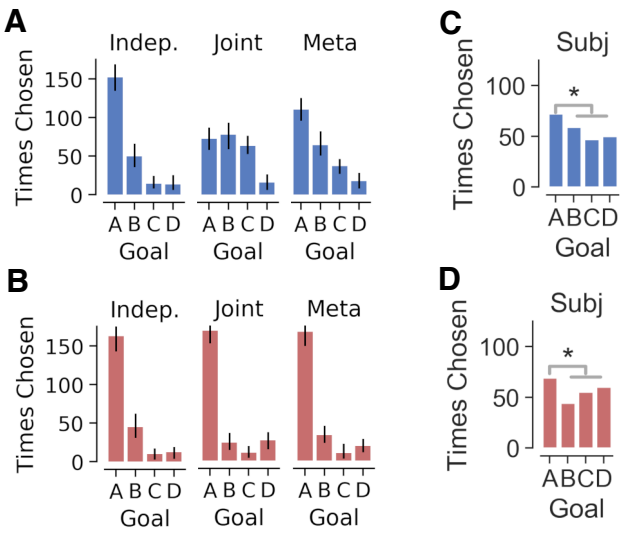

Figure 5. Goal selection in the first trial of novel test contexts in Experiment 2, separated by associated mapping transitions (blue and red). *A*, *B* Number of times each goal was selected by the independent, joint and meta computational agents in test contexts 1 & 2 (*A*), which shared the low-popularity transition (mapping) function, and in test contexts 3 & 4 (*B*), which shared the high-popularity transition function. *C*, *D* Like the independent agent, subjects chosen goal A more frequently than the other goals across both contexts.

B). Independent clustering predicts that goals will be chosen in these trials with the most popular goal selected most frequently, regardless of the associated mapping. In contrast, both the joint clustering and meta agents predict the goal selection in these trials will be influenced by the mapping. This leads to the qualitative prediction that in the first trial of test context 1 and 2, independent clustering and the meta-agent predict subjects will select goal A more often than either goals B or C, while joint clustering does not make this prediction.

Human Behavior. We analyzed the behavior of 114 subjects in experiment 3. As in the previous experiment, goal accuracy, reciprocal reaction time and navigation efficiency were assessed as a function of time using Bayesian linear modeling in order to verify learning during the training contexts. The number of trials per context was found to predict accuracy (Fig S3 A; $\mathbb{E}[\beta_t]$=0.115, 95% HPD = [0.108, 0.121]), reciprocal

reaction time ($\mathbb{E}[\beta_t] = 0.016$: 95% HPD = [0.014, 0.017]) and navigation efficiency ($\mathbb{E}[\beta_t] = -0.006$, 95% HPD = [-0.007, -0.005], indicating subject performance improved over the course of training.

Analysis of the *a priori* test context contrasts was consistent with the predictions of the independent clustering and meta agents. These contrasts were assessed with a hierarchical Bayesian logistic regression that included time with context, a subject specific bias term, and whether a trial of the same context sequentially followed a correct trial as nuisance variables (see *Materials and Methods*). Test accuracy was predicted by both nuisance factors and increased with the number of times a context was seen ($\mathbb{E}[\beta_t] = 0.48$, 95% HPD=[0.423, 0.553]) and when a trial of the same context was repeated sequentially ($\mathbb{E}[\beta_{\text{rep}}] = 0.923$, 95% HPD=[0.685, 0.164]).

Of the three contrasts, the difference between contexts 1 and 2 was statistically significant, (Fig 4 D; $\mathbb{E}[\beta_{1>2}] = 0.139$, HPD=[0.018, 0.274], $p_{\text{1-tail}} = 0.017$, 95% HPD = [0.011, 0.268]), whereas the other two contrasts were not statistically significant (context 1 & 2 vs 3 & 4: $\mathbb{E}[\beta_{1+2>3+4}] = 0.059$, HPD=[-0.024, 0.149] $p_{\text{1-tail}} = 0.102$; context 3 vs. 4: $\beta_{3>4}$:, 95% HPD = [-0.0068, 0.166]). Follow-up analyses suggested these effects were driven by positive transfer in test context 1. Accuracy was higher in test context 1 than 3 and 4 (context 1 vs 3 & 4: $\mathbb{E}[\beta_{1>2} + \beta_{1+2>3+4}] = 0.198$, 95% HPD = [0.045, 0.268]) but there was no difference between accuracy in test context 2 than in 3 and 4 (context 2 vs 3 & 4: $\mathbb{E}[\beta_{1+2>3+4} - \beta_{1>2}] = -0.080$, 95% HPD = [-0.235, 0.077]). Thus, accuracy in test context 1, which was associated with the most popular goal overall, was higher than in the other three contexts whereas we did not find a difference between the remaining test contexts. These results are consistent with generalization of the most popular goal overall (goal A) but not the parametric effects predicted by the models.

Subjects' goal selection in the first trial of a test context was also consistent with independent clustering and the meta-agent but not joint clustering. Goal choice was analyzed at a group level with two binomial models (*Materials & Methods*). Consistent with the predictions of independent clustering and the meta-agent, across all trials the choice-probability of goal A was above chance ($\mathbb{E}[\theta_A] = 0.309$, 95% HPD=[0.268, 0.353])

and higher than the average choice probability of goals B and C ($\mathbb{E}[\theta_A - \frac{1}{2}(\theta_B + \theta_C)] = 0.085$, 95% HPD=[0.034, 0.135]). Furthermore, this was true regardless of the associated mapping. Choice probability for goal A was greater than the average goal probability for goals B and C in contexts 1 and 2 (Fig 5C; $\mathbb{E}[\theta_A - \frac{1}{2}(\theta_B + \theta_C)] = 0.083$, 95% HPD=[0.009, 0.150]) and in test contexts 3 and 4 (Fig 5D;$\mathbb{E}[\theta_A - \frac{1}{2}(\theta_B + \theta_C)] = 0.087$, 95% HPD=[0.017, 0.157]).

Thus, we find evidence that subjects generalized the goal with the highest overall context popularity, regardless of the mapping presented in the context. We did not find evidence that goal generalization was parametrically proportional to context-popularity (e.g., preference for goal B over goal C or D), a prediction of all three models as a consequence of the CRP prior.

Experiment 3: Ambiguous structure

Experiments 1 and 2 showed that subjects generalization learning in novels contexts was more similar to a joint agent when the statistics of the training environment supported joint structure (experiment 1) and more like an independent agent when the statistics supported independent structure (experiment 2). In experiment 3, we provided subjects with a task environment with a more ambiguous relationship between mappings and goals in order to probe whether subjects would show evidence of both joint and independent clustering within the same task. This mixture of joint and independent clustering is a key prediction of the meta-agent, which is able to consider both forms of structure and to make inferences in novel environments that are influenced by the prior training statistics. Indeed, across both previous experiments, subjects behave more similarly to the meta agent than either joint or independent clustering alone, but we have not yet provided evidence for the meta-agent within a single task.

Thus, in the final experiment, we presented subjects with an environment with a more ambiguous relationship between goal-values and state-transitions across contexts (Fig 6). In this case, the joint vs. independent structure statistics were more

ambiguous: goal A was the most popular and paired with different mappings (consistent with independent structure), whereas goals B and C were always paired with a single mapping (consistent with joint structure). Furthermore, goal A was the most popular goal overall, but was equally popular to goal C conditional on experiencing the lower-popular mapping. As in the prior experiment, this design differentiates the predictions of independent and joint clustering, as the former is sensitive to the overall goal popularity whereas the latter is sensitive to the popularity conditioned on the associated transition function. Subjects completed 120 training trials across five contexts prior to completing 30 trials in four novel test contexts chosen to probe generalization (Fig 6A; Table S3).

This task has a more ambiguous relationship between mappings and goals than either experiment 1 or experiment 2. This is most clear in the mutual information between mappings and goals within the training contexts, which we normalize here by overall goal entropy for the purpose of cross-experiment comparison (see *Materials and Methods*). When normalized mutual information (NMI) is 1, there is a perfect correspondence between mappings and goals and when NMI is 0, there is no relationship. When we evaluate the training sets of each of the experiments, we see a correspondence between NMI and generalization strategy. In experiment 1, where we found evidence for joint clustering, the relationship between mappings and goals is strongest (Figure 7; NMI = 1.0). In experiment 2, where we found evidence for independent clustering, the relationship was the weakest (NMI $\approx$ 0.16). In experiment 3 the relationship between mappings and goals is somewhere between the other two experiments (NMI$\approx$ 0.3). As meta-agent updating is sensitive to the correspondence between mappings and goals (Franklin & Frank, 2018), we would thus expect more of a blend of joint and independent clustering in experiment 3.

As in experiment 2, there was no incentive to generalize, as confirmed by simulations showing that none of the three generalizing agents accumulated greater total reward than a non-generalizing "flat" agent during either the training or test contexts (all p's$<$.004 in favor of the flat model). We thus again designed the task such

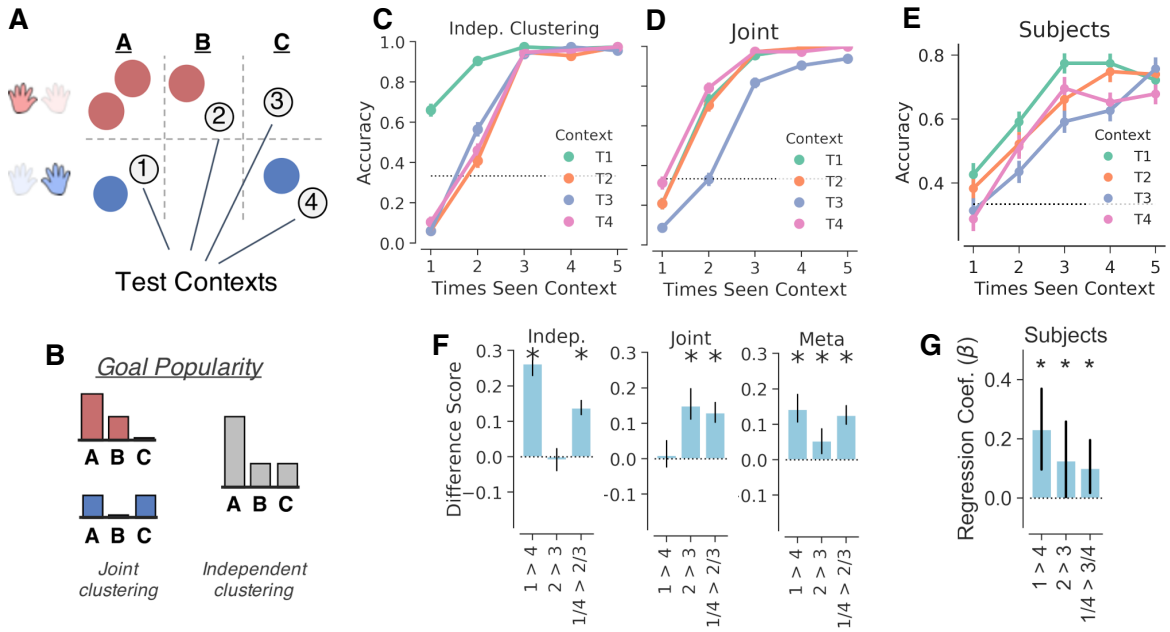

Figure 6. Experiment 3: Ambiguous structure. Subjects saw five contexts (circles) during training, each paired with one of two mappings (*red*: high popularity, *blue*: low popularity) and one of three goals (A, B, or C). The most popular goal A was paired with multiple mappings, but the other goals B and C were paired with a single mapping each, making the structure more ambiguous. Subjects learned to navigate in an additional four novel test contexts following training (grey circles). *B*: Goal popularity in the training environment as a function of mapping (as tracked by the joint agent, left) and collapsed across all contexts (as tracked by the independent agent, right). *C, D & E*: Test accuracy as a function of the number of trials in a context for the independent agent (*C*), joint agent (*D*), and subjects (*E*) Subject error bars reflect within-subject standard error. *F*: Qualitative model predictions expressed as difference scores between test contexts for the independent clustering, joint clustering, and the meta-agent. *G*: Group level regression weight of test context accuracy for subjects, who show patterns most like the meta agent (a mixture of joint and independent agents). Error bars reflect 95% HPD.

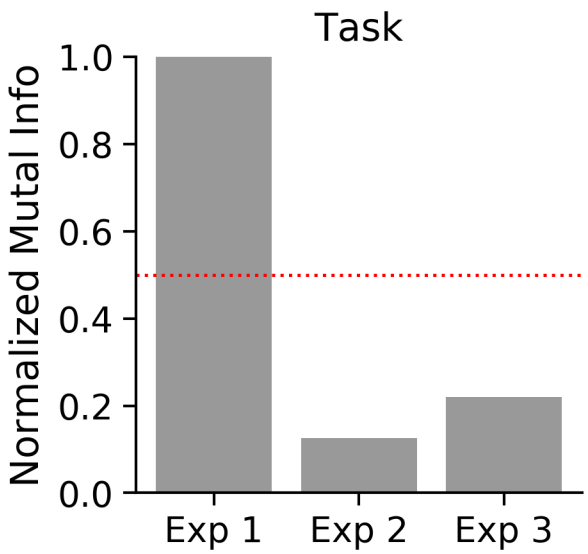

Figure 7. Left: Correspondence of mappings and goals across contexts for each experiment quantified with normalized Mutual information (NMI). Where NMI is close to 1, joint clustering is advantageous and when NMI is close to 0, independent clustering is advantageous.

that it was possible to discriminate between predictions of different types of generalization models without incentivizing generalization. Two comparisons, the contrast between test context 1 and 4 and the contrast between contexts 2 and 3, differentiate the predictions of joint and independent clustering. Test contexts 1 and 4 shared the low-popularity mapping and were paired with goals A and C, respectively. Goal A was the highest popularity goal overall but was equally popular to goal C when conditioned on the low-popularity mapping. Thus, the independent agent performs better in test context 1 compared to test context 4 (M=0.262, 95% HPD=[0.230, 0.295]), whereas the joint agent shows no such advantage (Fig 6 D, F; M=0.009, 95% HPD = [-0.023, 0.050]). Conversely, consider the contrast between test contexts 2 and 3, both of which were paired with the high-popularity mapping, but were associated with goals B and C, respectively. These two goals shared the same overall popularity but differed in popularity conditional on the high popularity mapping. As such, the joint clustering agent performs better in test context 2 than 3 (M=0.149, 95% HPD = [0.112, 0.198])), while independent clustering shows no difference (M=-0.008, 95% HPD

= [-0.039, 0.023]). Critically, the meta agent showed patterns consistent with both independent clustering (test context 1 > 4: M=0.142, 95% HPD = [0.107, 0.184]) and joint clustering (test context 2 > 3; M=0.053, 95% HPD = [0.018, 0.088]). For the purpose of completion, we also compare contexts 1 and 4 vs 2 and 3, affording three orthogonal contrasts for the regression model; all three models predicted a positive value for this difference (independent: M=0.138, 95% HPD = [0.119, 0.159]; joint: M=0.130, 95% HPD = [0.104, 0.159]; meta: M=0.123, 95% HPD = [0.101, 0.1152])

In sum, the three models make qualitatively different predictions. The joint model predicts a cost in test context 3; the independent model predicts an advantage in test context 1, and, given the ambiguity of the statistical structure during training, the meta model predicts a mixture of both effects (Fig 6).

Human Behavior. The behavior of 115 subjects was analyzed on the task. As for prior experiments, goal accuracy, reciprocal reaction time and navigation efficiency were assessed as a function of time using Bayesian linear modeling (see above and *Materials and Methods*). The number of trials per context was found to predict accuracy (Fig S2; $\mathbb{E}[\beta_t] = 0.109$, 95% HPD = [0.098, 0.012]), reciprocal reaction time ($\mathbb{E}[\beta_t] = 0.008$, 95% HPD = [0.0063, 0.0091]) and navigation efficiency ($\mathbb{E}[\beta_t] = -0.003$, 95% HPD = [-0.0043, -0.0027]), indicating subject performance improved over the course of training.

Accuracy in the test contexts provided support for the meta-learning agent over either the joint or independent clustering agent (Fig 6 E, G). Test context accuracy was assessed with hierarchical Bayesian logistic regression where the *a priori* model predictions were instantiated as contrasts between contexts (1 vs 4 and 2 vs 3), with the number of trials per context, and whether a context was sequentially repeated were included as nuisance regressors (*Materials and Methods*). Subjects' accuracy increased with the number of trials within each test context ($\mathbb{E}[\beta_t] = 0.43$; $p_{\text{1-tail}} < 0.0005$, 95% HPD = [0.36, 0.51]) and when a context was repeated on the next trial ($\mathbb{E}[\beta_{\text{rep}}] = 0.75$; $p_{\text{1-tail}} < 0.0005$, 95% HPD = [0.48, 1.01]). Critically, subjects were more accurate in test context 1 than 4 ($\mathbb{E}[\beta_{1>4}] = 0.232$, 95% HPD = [0.104, 0.367], $p_{\text{1-tail}} < 0.0005$) and were

more accurate in test context 2 than in 3 ($\mathbb{E}[\beta_{2>3}] = 0.123$, 95% HPD = [0.004, 0.258], $p_{\text{1-tail}} < 0.0275$). Subjects were also more accurate in contexts 1 and 4 than in 2 and 3 ($\mathbb{E}[\beta_{1+4>2+3}] = 0.102$, 95% HPD = [0.009, 0.188], $p_{\text{1-tail}} < 0.0125$).

As a follow up analysis, we further examined positive and negative transfer in the first trial of a test context (above or below chance performance on the first trial; Fig 6 C, D). Both independent clustering and the meta agent predict positive transfer in test context 1 and negative transfer in the other test contexts, given the overall popularity of goal A during training. Joint clustering does not predicts positive transfer in any context and predicts negative transfer in contexts 1, 2 and 3. Consistent with independent clustering we found positive transfer in test context 1 ($y \sim \text{Binom}(\theta)$; $\Pr(\theta_1 > \frac{1}{3}) = 0.963$, 95% HPD=[0.325, 0.500]) but did not find evidence of positive or negative transfer in the other test contexts ($y \sim \text{Binom}(\theta)$; θ_2: 95% HPD=[0.29, 0.46]; θ_3: 95% HPD=[0.23, 0.40]; θ_4: 95% HPD=[0.21, 0.38]).

Overall, these results are consistent with the predictions of the meta-agent and are not fully captured by either the independent or joint clustering agents.

Discussion

In the current work, we evaluated human generalization against the predictions of three dissociable computational models. The independent model assumes that subjects generalize in novel environments based on the overall popularity of the previous goal and mappings independently. The joint model assumes that subjects re-visit goal locations in proportion to how often they were paired with each mapping. Finally, the meta-generalization agent assumes that subjects learn the overal statistical relationship between goals and mappings and then generalizes based on the evidence for independent or joint structure. Across the suite of tasks, we provided evidence that humans vary their generalization strategy with the learned statistics of their environment in an adaptive way. In doing so, we replicated prior work demonstrating that human subjects exhibit positive transfer for previously learned task-sets (stimulus-response-outcome relationships; Collins et al., 2014; Collins & Frank, 2013),

with increasing generalization performance for those rules that had been most popular across training contexts (Collins & Frank, 2016). Even when popular contexts were experienced fewer times, subjects tended to generalize the goals associated with popular contexts, suggesting context popularity-based generalization, rather than raw frequency. Further, subjects generalized in experiments 2 and 3 even as it was disadvantageous, replicating the prior finding suggesting that humans will generalize spontaneously even if it requires paying a cost to do so (Collins, 2017; Collins & Frank, 2013).

However, prior empirical work assumed that task-sets are generalized as a whole, meaning that transitions and reward outcomes were linked as a single entity that can be reused, thus amounting to joint clustering. The current set of studies was thus designed to disrupt and manipulate the relationship between transition and reward functions. As predicted by theoretical work (Franklin & Frank, 2018), subjects were able to generalize each function independently of the other, particularly when the training environment was suggestive of such independent structure. These results provide evidence for the flexibility of human generalization, including the tendency to recombine component pieces of knowledge that have not been experienced together, to new contexts. For example, in experiments 2 and 3, like the independent model, subjects were more accurate at reaching the previously most popular goal A, even when it required using a less popular mapping. This situation is analogous to a musician that can transfer popular songs learned across multiple instruments to another instrument even with very different needed physical action requirements. However, when the task statistics implied joint structure, subjects were able to harness that relationship to generalize accordingly, repeating goals that had been previously paired with the same mapping over those that had been reached using a different mapping function (experiment 1 and partially experiment 3). This situation is analogous to exhibiting a preferential tendency to play a song on a new instrument which has shared actions required to produce the desired effect.

Why do we expect these tasks to produces these generalization strategies? If subjects are acting adaptively, then we would expect them to use the statistics of the

training set to inform the nature of their generalization strategy on the test set, thus amounting to a form of meta-generalization. This meta-generalization is normatively driven by the degree to which state transitions and rewards are mutually informative. In our three experiments, this relationship was the strongest in experiment 1 and weakest in experiment 2 (Figure 7); thus we would expect a normative generalization strategy consistent with joint clustering in experiment 1 and consistent with independent clustering in experiment 2.

In practice, the meta agent chooses its policy based on the degree to which joint or independent clustering has explained reward outcomes in the past. This is an approximation of the Bayesian model evidence of each generalization strategy (Franklin & Frank, 2018) and is similar to other value-based mechanisms proposed to arbitrate between model-free and model-based control (Kool, Cushman, & Gershman, 2016), the use of working memory vs. reinforcement learning(**?**), and to arbitrate amongst multiple "experts" for describing multidimensional hierarchical rules **?**. It is worth noting however, that the relative value of independent vs. joint clustering is not strictly equivalent to the mutual information between state transitions and rewards, and thus the meta agent strategy may deviate from what is predicted by mutual information. For example, the distribution of rewards across contexts will affect arbitration in the meta agent. Indeed, this is the case for in experiment 2, in which the meta agent predicts a higher probability of joint clustering than expected based on the mutual information in the task (Figure 8). While this is surprising, these tasks were not designed to compare multiple potential arbitration strategies, but instead to qualitatively differentiate between joint and independent clustering and test whether subject generalization appropriately reflects the statistics of the task.

From a normative perspective, independent clustering can be cast as a dimension reduction strategy, given that joint clustering requires learning covariance across multiple dimensions (Franklin & Frank, 2018). A similar point has been made in the context of whether subjects learn about entire objects as a whole (configural learning), or instead focus on individual features (Niv et al., 2015). Both independent clustering

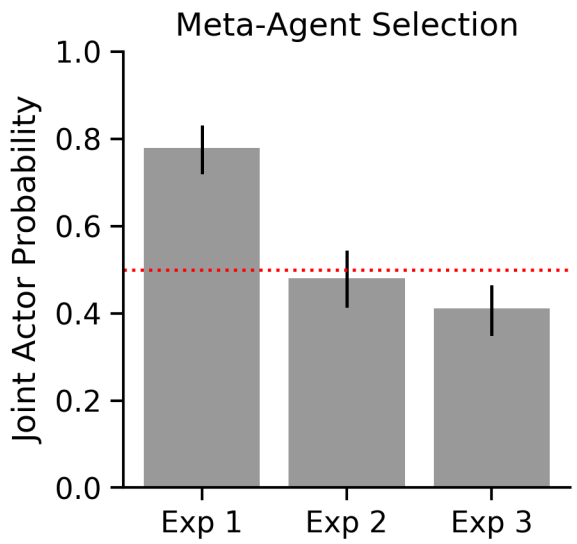

Figure 8. Meta-agent selection at the end of training. The meta-agent learns to probabilistically arbitrate between joint and independent clustering from experience. The probability the meta-agent selects the joint actor is shown for experiments 1 (joint structure), 2 (independent structure), and 3 (ambiguous structure).

and feature learning are strategies that reduce dimensionality by learning about one aspect of a task by marginalizing over all of the other properties, whereas joint clustering and configural learning are asymptotically unbiased. In reinforcement learning domains, humans learn about both individual features and configurations of features (Duncan, Doll, Daw, & Shohamy, 2018; Farashahi, Rowe, Aslami, Lee, & Soltani, 2017), and task demands appear to influence whether subjects learn about features or configurations (Melchers, Shanks, & Lachnit, 2008)

Mechanistically, learning about latent task-set structure is thought to involve the same, albeit hierarchically nested, frontostriatal circuits that are responsible for simple reward feedback-based learning (Collins et al., 2014; Collins & Frank, 2013, 2016). How might this circuitry adapt to assume joint vs independent clustering? One simple mechanism to enforce compositional representations of goals and transitions would be to embed them in independent systems. For example, learning motor mappings might involve interactions among basal ganglia, cerebellum and/or motor areas of the cortex (Doya, 1999; A. Fermin et al., 2010; A. S. Fermin et al., 2016), while learning

reward/goal values may involve interactions among prefrontal areas representing value and/or state (Bartra, McGuire, & Kable, 2013; Frank & Claus, 2006; Schuck, Cai, Wilson, & Niv, 2016; R. C. Wilson, Takahashi, Schoenbaum, & Niv, 2014). Thus the ventral striatal orbitofrontal circuit could learn goal or state values that can be reused independently of the actions needed to reach them (Frank & Claus, 2006; Padoa-Schioppa & Assad, 2006), thus potentially facilitating compositional recombination.

In contrast, when higher order rules or goal values are used to constrain physical mappings, such joint structure can be learned in hierarchical rostrocaudal circuits that embed multiple levels of abstraction (Badre & Frank, 2012; Collins & Frank, 2013; Frank & Badre, 2012). The mechanisms by which the brain could infer which of these structures (orthogonal/independent vs. hierarchical) should be used remain underexplored. Nevertheless, previous modeling and empirical work has suggested that reinforcement learning principles can be used to engage the level of rostrocaudal hierarchy needed for a given task, and when such hierarchy is not present, reward prediction errors are used to prevent gating of these circuits in favor of combinatorial representations (Badre & Frank, 2012; Frank & Badre, 2012). Indeed, these studies found that the degree of evidence of hierarchical structure using a Bayesian mixture of experts akin to our meta-learning agent, was related to the development of hierarchical gating policy in the neural network (Collins & Frank, 2013; Frank & Badre, 2012). More recent work has suggested this form of structure learning is neurally dissociable from the associative learning and involves the rostrolateral prefrontal cortex and angular gyrus (Tomov et al., 2018).

An open question is how compositional representations of goals and mappings can be combined to form a behavioral policy. In the above experiments, we were able to dissociate generalization of goals from mappings by dissociating learned goal-values from navigation with a multistep navigation task that enforced planning (A. Fermin et al., 2010; A. S. Fermin et al., 2016). Exact solutions to planning requires a system of equations and how this occurs is unknown and is a problem common to all model-based,

though several approximate planning algorithms have been proposed (but see Huys et al., 2012; Momennejad et al., 2017; Russek, Momennejad, Botvinick, Gershman, & Daw, 2017; Solway & Botvinick, 2012).

Limitations

While we found consistent evidence for the most diagnostic qualitative patterns predicted by the meta agent across three experiments, not all of the predictions of the model were borne out. Our models of generalization, like previous clustering models of generalization, rely on the CRP prior. When used in context-popularity based clustering, the CRP predicts that contexts will be generalized as a parametric function of their popularity. While previous data confirms that subjects do have a strong bias to prefer more popular structures as a prior Collins and Frank (2016), , that work did not assess whether such an effect was parametric (i.e. increasingly stronger preferences for increasingly more popular structures). We find mixed evidence for such a parametric effect in our data. In experiment 2, we found evidence that subjects generalize only the most popular goal. In experiment 3, two of the three significant test context contrasts relied on the distinction between the second and third most popular goal in training (specifically, the contrast between contexts 2 and 3 and the contrast between 1 and 4 vs 2 and 3 involved these preferences). Assuming this partial null effect does not simply reflect an absence of statistical power, there are multiple potential explanations, the most simple of which is that experiment 2 was more difficult than experiment 3 (as it had more training contexts and more goals to choose from) and consequently, subjects had lower accuracy in experiment 2 than in experiment 3 (Figure S4; experiment 2 vs 3: difference score = -0.045, $t=2.3$, $p<0.03$). Because subjects tend extend less cognitive effort in more demanding tasks (Kool, McGuire, Rosen, & Botvinick, 2010; Westbrook, Kester, & Braver, 2013), it is possible that relied on a less cognitively demanding strategy.

The difference in task complexity (which extends to the first experiment as well) resulted from experimental choices designed to increase the interpretability of the

experiments. Critically, the ability to resolve the predictions of joint and independent clustering is related to the complexity of the space of reward and mapping functions, as the models make different predictions only in explored regions of this space. We increased the space of contexts and goals in experiments 2 and 3 in order to differentiate model predictions on a within-subjects basis. In addition, we balanced the number of presentations of each context so as that each goal would be correct the same number of times. Otherwise, goals associated with higher popularity contexts would have a higher expected value marginalized across contexts. These two choices interact such that contexts were experienced less frequently in experiment 2 than experiment 3, increasing difficulty of the associative learning problem.

A further consequence of these choices is that working memory demands are not equal across the tasks. This consequently offers an alternative explanation to the meta-agent: people may be arbitrating their generalization strategy based on complexity of the task-space as opposed to reward prediction. How working memory would influence the arbitration strategy is not obvious, but intuitively, we might expect people to favor joint structure to the extent that working memory capacity supports it and then switch to independent structure as task complexity increases. Joint structure is more representationally greedy than independent structure, and such, we would expect it requires a higher memory load to learn the reward contingencies. Subjects learn reward contingencies more slowly under higher memory load (Collins & Frank, 2012) and we would expect working memory decay to affect joint and independent structure unequally. Joint clustering will necessarily result in at least as many context-clusters as independent clustering, meaning that the reward values of independent clustering are updated more frequently. In the context of the Bayesian agent we have presented, this difference is unimportant but if reward values are subject to working memory decay, than joint clustering may produce worse estimates of reward and thus, the meta-agent may favor independent clustering as task-complexity increases.

The question of how working memory demands influence generalization strategy is an open question for future research. More generally, we have considered the choice of

generalization strategy from a normative statistical perspective and have not considered resource constraints our model. These constraints are likely important; one reason learning compositional representations is valuable is they require fewer representational resources. In the context of clustering task structure, this corresponds to fewer numbers of context clusters. As such, we should expect resource demands and generalization strategy to tradeoff. Notwithstanding this potential explanation, it remains clear from our data that people arbitrate between a compositional and non-compositional generalization strategy depending on task demands.

Finally, in this study we presented model predictions and behavioral analyses at a group level and do not make claims about individual subjects. This limitation is a consequence of the task design: we probe generalization in a small number of test trials chosen to qualitatively differentiate the computational models. There are only a few (2-4) trials per subject per measure that distinguish the model predictions and most of the trials in each experiment are used to teach the subjects the statistics of the task or to balance the stimulus-action-outcome value of each goal and button-press. While we could attempt to fit a process model to each subject to determine each subject's generalization strategy, the estimated strategy of each subject will be highly dependent on a few trials and we are hesitant to rely this type of individual difference metric. However, this is not a limitation of the grouped data because of its larger sample size. The models make unique and identifiable qualitative predictions on these tasks and the metrics of these predictions, the context contrasts, are orthogonal from each other and not correlated with overall performance. As such, we believe it is strong to make qualitative predictions about which conditions show better or worse performance especially when the predicted patterns are orthogonal as here.

Materials and Methods

The code for our experimental design and all of our analyses and computational model are available online in our GitHub repository:
https://github.com/nicktfranklin/CompositionalGeneralization

Subjects

We collected in subjects online using Amazon mechanical turk and psiturk (Gureckis et al., 2016). All participants were compensated for their participation and gave informed consent as approved by the Human Research Protection Office of Brown University.

Experiment 1. 151 subjects completed experiment 1, two of which were excluded for reporting they took written notes during the experiment. Cluster analysis was used to assess non-performance on the task. A Gaussian mixture model was fit to two measures: the accuracy in trials following a correct trial of the same context and the binomial chance probability in all other training context trials (see *SI Materials and Methods*). Of the remaining 149 subjects, 34 were excluded on the basis of their performance on these measures.

Experiment 3. For experiment 3, we collected 153 subjects, five of which were excluded for reporting they took written notes. Using the same measures and analysis as in experiment 1, we used cluster analysis to excluded 33 subjects on the basis of their performance in the training contexts.

Experiment 2. 198 subjects completed the task, of which two subjects were excluded for reporting they took written notes during the experiment. Cluster analysis was used to asses subjects for non-performance. A Gaussian mixture model was fit to the two measures: trials following a correct trial of the same context and the overall accuracy in all other training context trials (see *SI Materials and Methods*). On the basis of this analysis, 67 subjects were excluded for non-performance.

Task

In each of the three experiments, subject controlled agent in a 6x6 grid world which they had to navigate into a labeled (‘A’, ‘B’, ‘C’, or ‘D’) goal location. In each study, subjects had to learn both the value of the goals in each context as well as a “mapping” between button responses (‘a’, ‘s’, ‘d’, ‘f’, ‘j’, ‘k’ , ‘l’, and ‘;’) and movement in the grid worlds (North, South, East, West). Each trial was a new instance of a grid

world and associated with a color-cued context. To aide memory, contexts were autocorrealted in time. In each context, one goal provided a fixed deterministic reward while all other goals were unrewarded. Separately, each context was also associated with one of two deterministic mapping. One mapping was always associated with left-hand keys on a standard US keyboard (‘a’, ‘s’, ‘d’, ‘f’) and the other was always associated with the right-hand keys (‘j’, ‘k’, ‘l’, ‘;’).

Subjects were required to learn both the identity of the correct goal and the mappings through exploration. To counterbalance for low level action-values, the location of the goals and the starting point of the agent were randomized on each trial. In addition, barriers were randomly placed in a subset of trials to encourage additional planning. The relationship between keypresses and movements was permuted across subjects, as was the visible label attached to each goal.

Subjects were instructed that each context was paired with a single mapping and a single rewarded goal location and asked to use their left-hand and right-hand to navigate. Subjects were instructed that the shared color of the agent and goal cued the mapping and the value of the goals and that this relationship was constant across all trials with the same color. As an additional memory cue in experiment 2, the each trial was labeled with a “room number” consistent with its context and all trials in a context within the experiment shared the same pattern of walls.

Computational Modeling

We used a version of the independent clustering, joint clustering and meta-agent models adapted from Franklin and Frank (2018) to generate qualitative predictions for each of the three experiments. Simulations were run generatively to inform the design of the experiments and make qualitative predictions. For the purpose of verifying the statistical significance of these predictions, we estimated the posterior distribution of the relevant comparisons via sampling. Specifically, we generated 1000 simulated samples of each model on each task and sub-sampled 200 batches of simulations matched to the sample size in the human experiments (e.g. for experiment 2, we

generated 200 batches of 115 simulations to match the 115 subjects collected). Accuracy, or binary rewards collected per trial, are reported as opposed to total reward.

Each model was a reinforcement learning model which learned a mapping function between keyboard responses and movements in the maze as well as a value function over goals. Formally, we define a mapping function with a probability mass function $\phi(a, A)$, where a defines a keyboard movement and A is a movement in the maze. As rewards in the task are binary, the value function over goals can also be expressed as a probability distribution over goals $R(g) = \Pr(g)$. For all three agents, mappings and goals are estimated with maximum likelihood estimation. Agents were provided with fully supervised information as to the attempted movement direction in the case the agent attempted to move through a barrier, as this information was visually signaled to human participants as well.

The mapping and reward function was constant and deterministic for all trials within a context. The models differed in how they assumed these functions were generalized across contexts. Joint clustering assumes that each context c belongs to a cluster of contexts k that share a single mapping and reward function, ϕ_k and R_k. Generalization is then cast as the problem of inferring the correct assignment of c into k via Bayesian inference:

$$\Pr(c \in k|\mathcal{D}) \propto \Pr(\mathcal{D}|k) \Pr(c \in k) \tag{1}$$

where the likelihood function $\Pr(\mathcal{D}|k) = \prod_{\mathcal{D}} \phi_k(A|a) R_k(g)$ is the product of the observed probability of a transitions and rewards on each trial for context cluster k. The prior is defined with a Chinese restaurant process (Aldous, 1985), defined

$$\Pr(c \in k) = \begin{cases} \frac{N_k}{N+\alpha} \\ \\ \frac{\alpha}{N+\alpha} \end{cases} \tag{2}$$

where N_k is the number of context previously assigned to a cluster, $N = \sum_k N_k$ is the total number of contexts visited thus far and α is a concentration parameter that governs the propensity for the process to assign a new context to a new cluster. For all of the simulations here, α was drawn from a standard log normal distribution, such that $\log \alpha \sim \mathcal{N}(-0.5, 1)$, to simulate individual differences generalization. During action

selection (discussed below) the *maximum a posteriori* (MAP) cluster assignment was used to approximate the posterior.

While joint clustering assumes mappings and goals generalize together, independent clustering loosens this assumption by assigning each context twice: once for mappings and once for goals. As before, cluster assignments are made via Bayesian inference (Eqn. 1) with the Chinese restaurant process prior (Eqn 2) but with a different likelihood for mapping clusters and reward clusters. Mapping clusters uses as their likelihood the mapping function $\Pr(\mathcal{D}|k) = \prod_{\mathcal{D}} \phi_k(A|a)$ whereas goal clusters use the reward function over goals as their likelihood $\Pr(\mathcal{D}|k) = \prod_{\mathcal{D}} R_k(g)$.

In contrast to both joint and independent clustering, the meta-agent does not employ a fixed generalization strategy and instead dynamically arbitrates between joint and independent clustering. This is done via sampling, where each strategy is sampled proportionally to how well it predicts reward in each novel context. Formally, each model is sampled according to its weight, w_m, which is defined as

$$w_m \propto \left(\prod_{t=1}^{n} \Pr(r_t|m) \right) \Pr(m) \tag{3}$$

where m is either independent or joint clustering and r_t is the reward observed on trial t. The prior over models, $\Pr(m)$, was chosen stochastically by sampling a uniform between zero and one. These model weights are an approximation of the unnormalized Bayesian model evidence and are consistent with a prediction error based arbitration strategy (Franklin & Frank, 2018). Thus, the meta-agent favors joint or independent clustering to the degree to it predicts unseen rewards.

Action selection was equivalent in all three models. Each agent had access to the structure of each grid-world on each trial in the form of a transition function $T(s, A, s')$. This transition function defined the probability of transitioning from location s to location s' having made the cardinal movement A. As movement in the grid-worlds was deterministic, this probability was always either one or zero. This was done to mirror human participants who have access to visual information indicating a spatial relationship between states as well as the locations of goals and the presence of barriers. We note that the spatial planning component of this task was intended to be simple for

human participants.

This transition function was used to solve an action-value function on each trial in terms of cardinal movements,

$$Q(s, A|c) = \sum_{s'} T(s, A, s') \left[R_{\hat{k}}(s') + V_{\hat{k}}(s')\right] \tag{4}$$

where $R_{\hat{k}}(s')$ is the reward function over states for the MAP cluster assignment $\hat{k}$ and where $V_{\hat{k}}$ is the corresponding value function over states. Here, the reward function $R_{\hat{k}}(s')$ is expressed over locations in the grid-world instead of over goals. In the behavioral task, goal locations are randomized to account for stimulus-response biases and the location of each goal is provided to the agent as it is visually available to subjects.

The value function over states, which defines the discounted expected reward of each state under the optimal policy, is defined by the Bellman equation,

$$V_{\hat{k}}(s) = \max_{A} \left[\sum_{s'} T(s, A, s') \left(R_{\hat{k}}(s') + \gamma V_{\hat{k}}(s')\right)\right] \tag{5}$$

where γ is a discount parameter set to $\gamma = 0.8$ for all agents. This system of equations is solved using value iteration (Sutton & Barto, 1998).

On each trial, a cardinal movement is sampled from a softmax function over the action-value function:

$$\Pr(A|s, c) \propto e^{\beta Q(s, A|c)} \tag{6}$$

where β controls the propensity to choose the highest valued action, set to $\beta = 10.0$ for all models to encourage greedy selection. The learned mapping functions were then used to sample keyboard responses,

$$\Pr(a|A) = \phi_{\hat{k}}(a|A) \tag{7}$$

Finally, an agent that did not generalize between contexts was used to assess the value of context-based generalization within the task by providing a performance baseline. This was done by assigning each context to it's own cluster. Conveniently, this can be interpreted as the limiting case of all of the generalizing agents with the concentration parameter α set to infinity and is thus otherwise the same.

Statistical Analyses

Hierachical Bayesian logistic regression. We analyzed test context accuracy in each of the three experiments with hierarchical Bayesian logistic regression (Gelman et al., 2014; Kruschke, 2014), with a hierarchical prior over individual regression coefficients. All models were estimated using the No-U-turn sampler, a variant of Hamiltonian MCMC (Hoffman & Gelman, 2011), implemented in the PyMC3 software library (Salvatier, Wiecki, & Fonnesbeck, 2016).

A priori model predictions were instantiated with and orthogonal set of contrasts between test contexts. Experiment 1 contained both within subjects and between subjects prediction and thus contained predictors for both. To control for within context learning, the number of trials in a context (t), whether a context was sequentially repeated (rep) were included as nuisance predictors. It was modeled with the following logistic regression model:

$$\text{logit}(p) = \beta_{\text{s}} S + \beta_H H \ + \beta_t t + \beta_{rep}\text{rep} \tag{8}$$

where $S \in \{0, 1\}$ is equal to 1 for the (between subjects) "Switch" condition, where "H"$\in \{0, 1\}$ is equal to 1 when the rewarded goal for the context is the high popularity goal. A hierarchical prior $\beta \sim \mathcal{N}(\mu_\beta, \sigma_\beta)$ was used for all predictors with a vague normal $\mu_\beta \sim \mathcal{N}(0, 100)$ and Cauchy hyper-prior $\sigma_\beta \sim \text{Half-Cauchy}(0, 100)$ for the mean and variance of each predictor, respectively.

The predictions of interest in experiments 2 and 3 were all within subjects measures. As both experiments had 4 test contexts, a maximum of three orthogonal contrasts were possible. As before, the number of trials in a context, whether a context was repeated were included as nuisance predictors. These were modeled as a linear combination of terms in a logistic regression,

$$\text{logit}(p) = \sum_c \beta_c c + \beta_t t + \beta_{rep}\text{rep} \tag{9}$$

where $\text{logit}(x) = 1/(1 + \exp(-x))$, c is a contrast, t is the trial number within a context and rep $\in \{0, 1\}$ indicates whether a context has been sequentially repeated.

Hierarchical priors for the regression coefficients were defined in the same manner as experiment 1.

Parameter estimates of the mean value μ_β were interpreted as group level effects and statistical significance was determined by gauging whether 0 fell within the 95% highest posterior density interval (HPD; Kruschke, 2014) or using a 1-tailed test, denoted as $p_{\text{1-tail}}$, where appropriate. An advantage of this Bayesian approach is that we are able to define novel contrast with the same posterior sample through algebraic manipulation (i.e. addition or subtraction) of our parameters. For additional insight, we report relevant contrast created through this form of recombination.

Analysis of goal selection. In experiment 2, we analyzed the probability each goal was chosen in the first trial of a novel context at a group level with two Bernoulli models. For the first model, we collapsed the goal selection for all subjects across all test contexts, and modeled the goal-choice probability with independent Bernoulli distributions,

$$p_g \sim \text{Bernoulli}(\theta_g) \tag{10}$$

where $g \in \{A, B, C, D\}$ is a goal. In a separate analysis, we modeled goal choice probability as independent Bernoulli distributions, collapsing across all test contexts that shared a transition function. Thus, as test contexts 1 and 2 shared the same transition function, θ_g was modeled modeled separately for contexts 1 and 2 than 3 and 4.

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Supporting information

Subject Exclusion Criteria

Our subject pool was recruited online using Amazon's Mechanical Turk platform. In order to control for the possibility some subjects were not engaged in the task and instead rushed through it as quickly as possible, we used subject performance on the training contexts to identify non-performance on the task. In experiments 2 and 3, we used two measures of performance during training: (1) accuracy on trials in which the preceding trial shared the same context and in which the subject responded correctly and (2) the probability subject goal-selection accuracy was at chance in all other trials, according to a binomial model. A Gaussian mixture model were fit to these two measures, we allowed the number of clusters to range between one and three and allowed for the and allowed for constraints over the covariance matrix to vary from spherical, diagonal, tied or full. Bayesian information criterion (BIC) was used for model selection, and the model with the lowest BIC was chosen. For both experiments 2 and 3, a model with 2 components and a diagonal constraint on the covariance matrix had the lowest BIC (Figure S1)

The members of the largest cluster were carried forward for analysis and all other subjects were used excluded. Follow up analyses found the excluded subjects were more likely to choose the goal closest to the initial location in each trial in both experiment 2 (Fig S1F; $t(65.8) = -6.4$, $p < 3 \times 10^{-8}$) and experiment 3 (Fig S1B; $t(42.8) = -7.1$, $p < 9 \times 10^{-9}$). In experiment 3, excluded subjects tended to rate the experiment as more difficult (Fig S1C; $t(47.6) = -4.3$, $p = 9 \times 10^{-5}$) and spent significantly more time viewing the instructions (Fig S1D; $t(45.1) = 3.5$, $p = 0.0011$). Neither of these two effects were present in experiment 1 (Fig S1G, H; difficulty: $t(53.3) = 0.76$, $p > 0.4$, viewing time: $t(57.7) = 0.30$, $p > 0.7$)

A similar clustering procedure was used to determine the subjects in experiment 1 that were carried through for further analysis but with loosened criteria as a large number of subjects were found to be excluded using the criteria above. This was likely due task differences as experiment three was substantially easier that the other two

tasks. Accuracy in trials in which the context was sequentially repeated and in which the previous trial was correct was again used as a dimension of the clustering analysis. In lieu of the binomial probability that all other trials were at chance accuracy, the raw accuracy in these trials was used. Chance accuracy in experiment 3 was 50%, and this was found to be too strict of a criterion. Subjects excluded in were less likely to choose the closest goal closest to the initial location of the agent ($t(115, 5) = -1.99, p = 0.049$) but we saw no difference in the time spent viewing instructions ($t(150.6) = 0.82, p > 0.4$, cohen's d $= 0.87$) or in rated task difficulty ($t(106.5) = -0.29, p > 0.7$)

Statistical analysis of training contexts

While performance in the training context was not directly of interest, generalization depends on learning the statistics of the training environment. We assessed three measures of learning as a function of time in the training contexts: goal-choice accuracy, reciprocal reaction-time and navigation efficiency, where navigation efficiency was defined as the number of steps taken in a trial minus the minimum path length required to reach the chosen goal. Each measure was analyzed using a hierarchical Bayesian general linear model:

$$f(x) = \alpha_{\text{subj}} + \beta_t * t + \beta_t t + \beta_{\text{rep}} \text{rep} \tag{11}$$

where x is the measure of interest, f is the linking function, t is the number of trials observed within a context, rep $\in 0, 1$ is an indicator function for whether the previous trial was correct and shared the same context and α_{subj} is a subject specific bias term (Kruschke, 2014). For accuracy, we used a logistic function as a linking function, for reciprocal reaction time we use a linear linking function (Noorani & Carpenter, 2016), and for navigation efficiency we use a Poisson linking function.

For the accuracy and reaction time analysis, we further assumed the hierarchical priors $\alpha_{\text{subj}} \sim \mathcal{N}(\mu_\alpha, \sigma_\alpha)$, $\beta_t \sim \mathcal{N}(0, 100)$ and $\beta_{\text{rep}} \sim \mathcal{N}(0, 100)$, with the weakly informative hyper-prior $\mu_\alpha \sim \mathcal{N}(0, 100)$, $\sigma_\alpha \sim \mathcal{N}(0, 100)$. For the navigation efficiency analysis, we used the stronger priors of $\beta_t \sim \mathcal{N}(0, 10)$ and $\beta_{\text{rep}} \sim \mathcal{N}(0, 10)$ as priors,

with the weakly informative hyper-prior $\mu_\alpha \sim \mathcal{N}(0,5)$, $\sigma_\alpha \sim \mathcal{N}(0,5)$ as the less informative priors failed to converge, likely due to the Poisson link function.

Non-zero values of β_t were interpreted as learning across time while all other predictors were considered nuisance parameters. The analysis of goal accuracy was also used to compare experiments, with the hierarchical mean over subject intercepts, μ_α, as a metric of group-level accuracy in the task.

Comparison between experiments

In this section, we examine the degree to which goals and mappings are related in the training contexts. We formalize this with normalized mutual information (NMI), which we define as

$$\text{NMI} = 1 - \frac{H(G|M)}{H(G)} \tag{12}$$

where $H(G|M)$ is the conditional entropy of the goals given the mapping and $H(G)$ is the marginal entropy of the goals. Both the conditional and marginal entropy are defined in bits as

$$H(G) = -\sum_g p_g \log_2 p_g \tag{13}$$

and

$$H(G|M) = -\frac{1}{N_m} \sum_{g,m} p_{g|m} \log_2 p_{g|m} \tag{14}$$

where p_g is defined as the frequency goal g is the correct goal in the training context, $p_{g|m}$ is the frequency goal g is the correct goal conditioned on mapping m and N_m is the total number of mappings.

For example, in experiment 1, there are three training contexts, two of which have "A" as the correct goal and one of which has "B." Therefore, $H(G) = -\left(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3}\right) \approx 0.92$bits. Because there is a perfect correspondence between mappings and goals in experiment 1, $H(G|M) = 0$ and consequently, NMI=1.

Context	Goal	Mapping	n Trials
Train 1	A	High Pop	8
Train 2	A	High Pop	8
Train 3	B	Low Pop	16
Repeat Test 1	A	High Pop	4
Repeat Test 2	A	High Pop	4
Repeat Test 3	B	Low Pop	8
Switch Test 1	A	Low Pop	4
Switch Test 2	A	Low Pop	4
Switch Test 3	B	High Pop	8

Table S1

Experiment 1: The number of trials within each context is balanced such that each goal and each mapping is presented the same number of trials across both training and test. Subjects saw either the "Repeat Test" context or the "Switch Test" contexts.

Context	Goal	Mapping Popularity	n Trials
Train 1	A	Low	20
Train 2	A	High	10
Train 3	A	High	10
Train 4	B	Low	20
Train 5	B	High	20
Train 6	C	Low	40
Train 7	D	High	40
Test 1	A	Low	6
Test 2	B	Low	6
Test 3	C	High	6
Test 4	D	High	6

Table S2

Experiment 2 task design. The number of trials within each context is balanced such that each goal and each mapping is presented the same number of trials across both training and test.

Context	Goal	Mapping Popularity	n Trials
Train 1	A	High	10
Train 2	A	High	10
Train 3	A	Low	20
Train 4	B	High	40
Train 5	C	Low	40
Test 1	A	Low	10
Test 2	B	High	10
Test 3	C	High	5
Test 4	C	Low	5

Table S3

Experiment 3 Task design. The number of trials within each context is balanced such that each goal and each mapping is presented the same number of trials across both training and test.

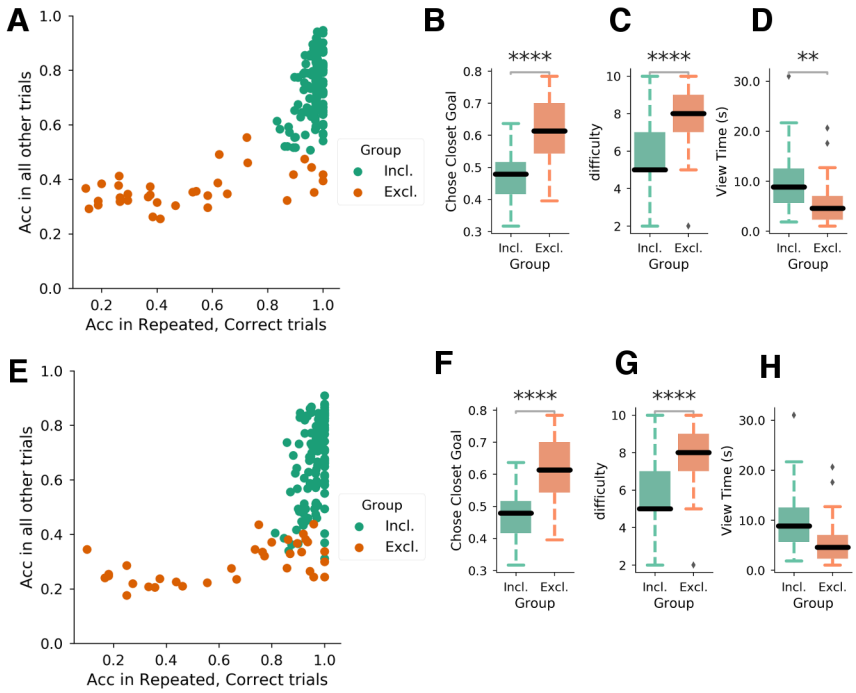

Figure S1. Cluster analysis of subjects training performance in experiments 1 (*A*-*D*) and 2 (*E*-*H*). *A*,*E*: Accuracy in repeated, correct trails vs all other trials. *B*,*F*: Proportion of time the closest goal was selected by inclusion status. *C*,*G*: Subject rated difficulty by inclusion status. *D*,*H*: Time spend reading viewing instructions by inclusion status

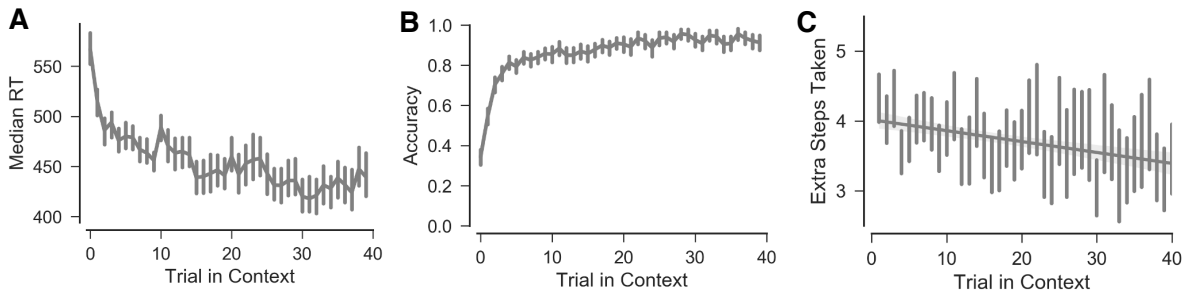

Figure S2. Experiment 1, Training performance. Accuracy (*A*), median reaction time (*B*) and the excess number of steps taken over the shortest path (*C*) shown as a function of the number of trials within each training context

Figure S3. Experiment 2, Training performance. Accuracy (A), median reaction time (B) and the excess number of steps taken over the shortest path (C) shown as a function of the number of trials within each training context

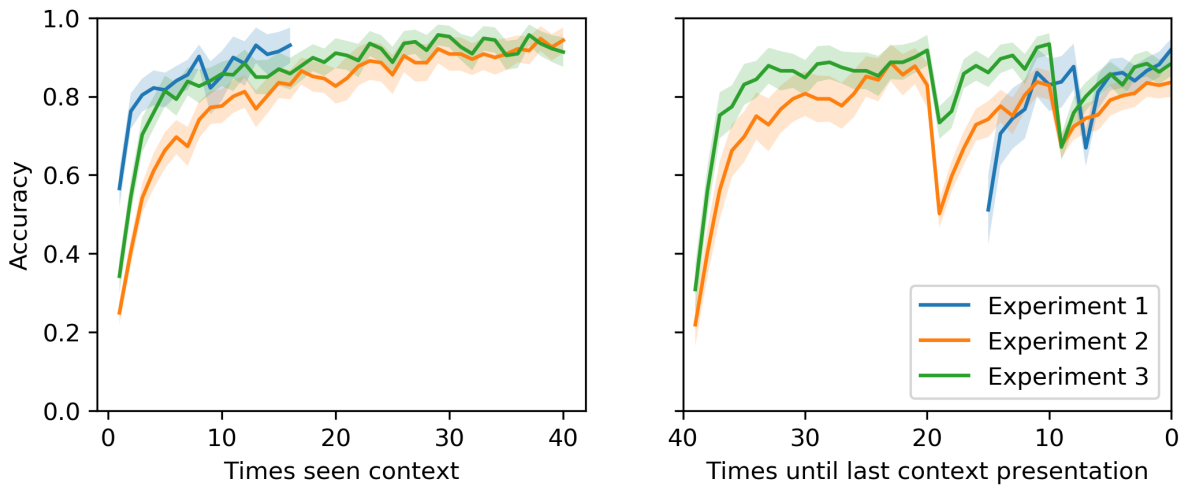

Figure S4. **Cross experiment training accuracy** *Left*: Accuracy as a function of the number of presentations in each context. Initial differences reflect a difference in chance accuracy between experiments *Right*: Accuracy as a function of number of presentations remaining (per context) within the training phase. Sharp drops in accuracy reflect the fact that each context was not shown the same number of times.