One Network, Many Robots: 
Generative Graphical Inverse Kinematics

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Abstract

Quickly and reliably finding accurate inverse kinematics (IK) solutions remains a challenging problem for robotic manipulation. Existing numerical solvers are broadly applicable, but rely on local search techniques to manage highly non-convex objective functions. Recently, learning-based approaches have shown promise as a means to generate fast and accurate IK results; learned solvers can easily be integrated with other learning algorithms in end-to-end systems. However, learning-based methods have an Achilles’ heel: each robot of interest requires a specialized model which must be trained from scratch. To address this key shortcoming, we investigate a novel distance-geometric robot representation coupled with a graph structure that allows us to leverage the flexibility of graph neural networks (GNNs). We use this approach to train the first learned generative graphical inverse kinematics (GGIK) solver that is, crucially, “robot-agnostic”—a single model is able to provide IK solutions for a variety of different robots. Additionally, the generative nature of GGIK allows the solver to produce a large number of diverse solutions in parallel with minimal additional computation time, making it appropriate for applications such as sampling-based motion planning. Finally, GGIK can complement local IK solvers by providing reliable initializations. These advantages, as well as the ability to use task-relevant priors and to continuously improve with new data, suggest that GGIK has the potential to be a key component of flexible, learning-based robotic manipulation systems.

1 Introduction

Robotic manipulation tasks are naturally defined in terms of end-effector positions and poses (e.g., for bin-picking or path following). The configuration of a manipulator is typically specified in terms of joint angles, however, and determining the joint configuration(s) that correspond to a given end-effector pose requires solving the inverse kinematics (IK) problem. For redundant manipulators (i.e., those with more than six degrees of freedom or DOF), every pose is reachable by an infinite non-convex set of feasible configurations. While redundancy allows high-level algorithms (for, e.g., motion planning) to choose configurations that best fit the overall task, it makes IK substantially more involved.

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Since the full set of IK solutions cannot be derived analytically in general for redundant manipulators, individual configurations reaching a target pose are found by locally searching the configuration space using numerical optimization methods and geometric heuristics. The search space is reduced by setting relevant parameters with the goal of finding solutions that have particular properties (e.g., collision avoidance, manipulability). This approach is limited by the local nature of the search as well as the capacity of individual methods to express desired properties. These limitations have motivated the use of learned models that approximate the feasible set, which may be used independently as IK solvers or to provide an initialization for a local search.

In terms of success rate, learned models that output individual solutions are able to compete with the best numerical IK solvers when high accuracy is not required [1]. Data-driven methods are also useful for integrating abstract criteria such as “human-like” poses or motions [2]. Generative approaches [3, 4] have demonstrated the ability to rapidly produce a large number of approximate IK solutions and even to model the entire feasible set for specific robots [5]. Access to a large number of configurations fitting desired constraints has proven beneficial in motion planning applications [6]. Unfortunately, these learned models, parameterized by deep neural networks (DNNs), require specific configuration and end-effector input-output vector pairs for training (by design). In turn, it is not possible to generalize learned solutions to robots that vary in link geometry and DOF. Ultimately, this drawback limits the utility of learning for IK over well-established numerical methods that are easier to implement and to generalize [7].

In contrast to existing DNN-based approaches [3, 6, 1, 4, 5], we explore a new path towards learning generalized IK by adopting a graphical model of robot kinematics [8, 9]. This graph-based description allows us to make use of graph neural networks (GNNs) and to incorporate appropriate relational inductive biases in the form of specific architectural assumptions [10] that capture varying robot geometries and DOF. GNNs have been employed to learn object manipulation policies that generalize to tasks with a greater number of objects than seen during training [11] and to varying agent structures [12, 13]. Motivated by the performance of generative models, our architecture leverages the proven capacity of conditional variational autoencoders (CVAEs) to represent diverse solution sets [14]. In this paper, we describe our generative graphical inverse kinematics (GGIK) model and explain its capacity for representing general (i.e., not tied to a single robot model) IK mappings. Remarkably, our results show that a single GGIK model is able to provide reasonable approximations of IK solutions for multiple robot manipulators with varying geometry. Our ambitious long-term vision for GGIK is, ultimately, to have a single trained model that can provide many diverse (approximate) solutions quickly and in parallel for a wide range of manipulators. This would enable what we call “shotgun IK” for sampling-based motion planning, manipulator design and workspace evaluation, and other IK applications, for example, where the model could be used in a “plug and play” manner. We hope that this work provides a baseline and lays down some foundation for learned general IK. Our code and models are open source.

2 Related Work

Inverse Kinematics Robotic manipulators with six or fewer DOF can reach any feasible end-effector pose [15] with up to sixteen different configurations that can be determined analytically [16, 17] or found automatically using the IKFast algorithm [18]. However, analytically solving IK for redundant manipulators is generally infeasible, and numerical optimization methods or geometric heuristics must be used instead. Simple instances of the IK problem involving small changes in the end-effector pose (e.g., kinematic control or reactive planning), also known as differential IK, can be reliably solved by computing required configuration changes using a first-order Taylor series expansion of the manipulator’s forward kinematics [19, 20]. As an extension of this approach, the infinite solution space afforded by redundant DOF can be used to optimize secondary objectives such as avoiding joint limits through redundancy resolution techniques [21]. By incrementally “guiding” the end-effector in the task space [22], this approach can also be used to find configurations reaching end-effector poses far from the starting configuration (e.g., a pose enabling a desired grasp). However, these closed-loop IK [23] techniques are particularly vulnerable to singularities and require a user-specified end-effector path reaching the goal.

1 Link to GitHub repository to be released after final CoRL accept/reject decisions.
The “assumption-free” IK problem that appears in applications such as motion planning is best solved using first-order [24, 7] and second-order [25, 26] nonlinear programming methods formulated over joint angles. These methods have robust theoretical underpinnings [27] and can approximately support a wide range of constraints through the addition of penalties to the cost function [7]. However, the highly nonlinear nature of the problem makes them susceptible to local minima, often requiring multiple initial guesses before returning a feasible configuration, if at all. These issues can sometimes be circumvented through the use of heuristics such as the cyclic coordinate descent (CCD) algorithm [28], which iteratively adjusts joint angles using simple geometric expressions, or the FABRIK [29] algorithm, which solves the IK problem using iterative forward-backward passes over joint positions to quickly produce high-quality solutions.

Some approaches forgo the joint angle parametrization in favour of Cartesian coordinates and geometric representations [30]. Dai et al. [31] use a Cartesian parameterization together with a piecewise-convex relaxation of SO(3) to formulate IK as a mixed-integer linear program, while Yenamandra et al. [32] use a similar relaxation to formulate IK as a semidefinite program. Naour et al. [33] express IK as a nonlinear program over inter-point distances, showing that solutions can be recovered for unconstrained articulated bodies. The distance-geometric robot model introduced in [8] was used in [9, 34] to produce Riemannian and convex optimization-based IK formulations. Our architecture adopts this paradigm to construct a graphical representation of the IK problem that can be leveraged by GNNs.

Learning Inverse Kinematics  Jordan and Rumelhart show in [35] that the non-uniqueness of IK solutions presents a major difficulty for learning algorithms, which often yield erroneous models that “average” the non-convex feasible set. D’Souza et al. [36] address this problem for differential IK by observing that the set of solution angle changes is locally convex around particular configurations. Bocsi et al. [37] use an SVM to parameterize a quadratic program, whose solutions match those of position-only IK for particular workspace regions. In computer graphics, Villegas et al. [38] apply an RNN model to solve a highly constrained IK instance for motion transfer between skeletons with different bone lengths. We show that a GNN-based IK solver allows a higher degree of generalization that captures not only different link lengths, but also different numbers of DOF.

Recently, generative models have shown potential to capture the full set of IK solutions. A number of invertible architectures [39, 14] have been able to successfully learn the feasible set of 2D kinematic chains. Generative adversarial networks (GANs) have been applied to learn the inverse kinematics and dynamics of an 8-DOF robot [3] and improve motion planning performance by sampling configurations constrained by link positions and (partial) orientations [6]. Recently, Ho et al. [4] proposed a model that retrieves configurations reaching a target position by decoding posture indices for the closest position in the database of positions. Finally, Ames et al. [5] describe a model that relies on normalizing flows to generate a distribution of IK solutions for a desired end-effector pose. Our architecture differs from previous work by allowing the learned distribution to be generalized to a large class of robots, removing the requirement of training a new model for each specific robot.

Learning for Motion Planning  Recent work has also investigated learning for classical motion planning problems. Prior applications of learning include warm-starting optimization-based methods [40], learning distributions for sampling-based algorithms [41, 42], and directly learning a motion planner [43]. While the methodology of our work is similar in some respects, we are interested in the IK problem and not in motion planning (i.e., trajectory generation). IK introduces additional challenges from the perspective of learning: capturing multiple solutions and handling multiple manipulators.

3 Preliminaries

3.1 Forward and Inverse Kinematics

Most robotic manipulators are modelled as kinematic chains composed of revolute joints connected by rigid links. The joint angles are arranged in a vector \( \theta \in C \), where \( C \subseteq \mathbb{R}^n \) is known as the configuration space. Analogously, coordinates \( \tau \) related to the task being performed constitute the task space \( T \). The forward kinematics function \( F : C \rightarrow T \) maps joint angles \( \theta \) to task space coordinates \( F(\theta) = \tau \in T \) of a robot, which can be derived in closed form using structural information (e.g., joint screws [44] or DH parameters [45]). We focus on the task space \( T := SE(3) \) of 6-DOF end-effector poses.
The inverse mapping $F^{-1} : T \rightarrow C$ defines the inverse kinematics of the robot. $F^{-1}$ is generally not unique (i.e., $F$ is not injective and therefore multiple feasible configurations exist for a single target pose $T \in \text{SE}(3)$). In this paper, we solve the associated problem of determining this mapping for manipulators with $n > 6$ DOF, where each end-effector pose corresponds to a set of configurations

$$IK(T) = \{\theta \in C \mid F(\theta) = T\}$$

that we refer to as the full set of IK solutions. Instead of finding individual configurations that satisfy the forward kinematics equations by performing a local search on problems with feasible sets $\mathcal{Q} \subset IK(T)$, we approximate $IK(T)$ itself as a learned conditional distribution in a higher-dimensional space.

### 3.2 Distance-Geometric Graph Representation of Robots

We eschew the common angle-based representation of the configuration space in favour of a distance-geometric model of robotic manipulators comprised of revolute joints [8]. This allows us to represent configurations $\theta$ as complete graphs $G = (V, E)$, whose edges $E$ are assigned non-negative weights $d_{u,v} \in \mathbb{R}^D$ indexed by vertices $V$, where $D \in \{2, 3\}$ is the workspace dimension. The coordinates of points corresponding to these distances are recovered by solving the distance geometry problem (DGP):

**Distance Geometry Problem** ([46]). Given an integer $D > 0$, a set of vertices $V$, and a simple undirected graph $G = (V, E)$ whose edges $\{u, v\} \in E$ are assigned non-negative weights $d_{u,v} \in \mathbb{R}_+$, find a function $p : V \rightarrow \mathbb{R}^D$ such that the Euclidean distances between neighbouring vertices match their edges’ weights (i.e., $\forall \{u, v\} \in E, \|p(u) - p(v)\| = d_{u,v}$).

It was shown in [9] that any solution $p \in \text{DGP}(\tilde{G})$ may be mapped to a unique corresponding configuration $\theta$. Crucially, this allows us to construct a partial graph $\tilde{G} = (V, E)$, with $E \subset E$ corresponding to distances defined by an end-effector pose $T$ and the robot’s structure (i.e., those shared by $IK(T)$) where all $p \in \text{DGP}(\tilde{G})$ correspond to particular IK solutions $\theta \in IK(T)$.

The generic procedure for constructing $\tilde{G}$ is demonstrated for a simple manipulator in Fig.1. First, the structure graph $G_s = (V_s, E_s)$ shown in Fig.1c is built by attaching two pairs of points labeled by vertices $u, \tilde{u}$ and $v, \tilde{v}$ to the rotation axes of neighbouring joints at a unit distance, as shown in Fig.1b. The edges associated with every combination of points are then weighted by their respective distance, which is determined solely by the link geometry, and the process is repeated for every pair of neighbouring joints. The resulting set of vertices $V_s$ and edges $E_s$, shown in Fig.1c, describe the overall geometry and DOF of the robot and are invariant to feasible motions of the robot (i.e., they remain constant in spite of changes to the configuration $\theta$). In order to uniquely specify points with known positions (i.e., end-effectors) in terms of distances, we define the “base vertices” $V_b = \{o, \bar{x}, \bar{y}, \bar{z}\}$, where $\bar{x}, \bar{z}$ are the vertices in $V_s$ associated with the base joint. Setting the distances weighting the edges $E_b$ such that they form a coordinate frame with $o$ as the origin, we specify edges $E_p$ weighted by distances between vertices in $V_p \subset V_s$ associated with the end-effector and the base vertices $V_b$. The resulting subgraph $G_e(V_b \cup V_p, E_b \cup E_p)$, shown in Fig.1d, uniquely specifies an end-effector pose under the assumption of unconstrained rotation of the final joint, while $\tilde{G} = G_s \cup G_e$ is the partial graph that uniquely specifies the associated IK problem.

\[ \text{Up to any Euclidean transformation of } p, \text{ since distances remain unchanged.} \]
Figure 2: Our GGIK solver is based on the CVAE framework. GNN_{enc} encodes a complete graph representation of a manipulator into a latent graph representation and GNN_{dec} “reconstructs” it. The prior network, GNN_{prior}, encodes the partial graph into a latent embedding that is near the embedding of the full graph. At test time, we decode the latent embedding of a partial graph into a complete graph to generate a solution.

4 Method

Our goal is to learn an inverse kinematics solver that is, crucially, capable of producing multiple diverse solutions while generalizing across robots. In the following subsections, we cover our data generation process, learning procedure, and network architecture in detail.

4.1 Dataset

To train our GGIK model, we require a dataset of partial graphs \( \tilde{G} \) and associated complete graphs \( G \). Conveniently, acquiring training data is fast and simple—any valid configuration can be used for training. We sample joint angles of various manipulators and use forward kinematics to obtain the end-effector pose. From the known robot geometry, end-effector pose, and joint angles, we are able to produce undirected graphs \( \tilde{G} = (V, \tilde{E}) \) and \( G = (V, E) \) with the procedure outlined in Section 3.2. For a complete graph \( G \), we define node features as a combination of point positions \( p = \{ p_i \}_{i=1}^N \in \mathbb{R}^{N \times D} \) and general features \( h = \{ h_i \}_{i=1}^N \), where each \( h_i \) is a feature vector containing extra information about each node. For GGIK, we use a three-dimensional one-hot-encoding, \( h_i \in \{0,1\}^3 \) and \( \sum_{j=1}^3 h_{i,j} = 1 \), that indicates whether the node defines the base coordinate system, a general joint or link, or the end-effector. In future work, we plan to add an extra class or dimension to indicate nodes that represent obstacles in the task space. Similarly, we can define the \( M \) known point positions of the partial graph \( \tilde{G} \) as \( \tilde{p} = \{ \tilde{p}_i \}_{i=1}^M \in \mathbb{R}^{M \times D} \) and set the remaining unknown \( N - M \) node positions to zero. The partial graph shares the same general features \( h = \{ h_i \}_{i=1}^N \) as the complete graph, given that we know which part of the robot each node belongs to in advance.

4.2 Learning to Generate Inverse Kinematics Solutions

We consider the problem of modelling complete graphs corresponding to IK solutions given partial graphs that define the problem instance (i.e., the robot’s geometric information and the task space goal pose). Intuitively, we would like our network to map or “complete” partial graphs into full graphs. Since multiple or infinite joint configuration solutions may exist for a single task space goal and robot architecture, a single partial graph may be associated with multiple or even infinite valid complete graphs. Having said this, we interpret the learning problem through the lens of generative modelling and treat the solution space as a multimodal distribution conditioned on a single problem instance. By sampling this distribution, we can generate diverse solutions.

At its core, GGIK is a CVAE model [47] that parameterizes the conditional distribution \( p(G | \tilde{G}) \) using GNNs. By introducing a stochastic latent variable \( z \), our generative model is

\[
p_{\theta}(G | \tilde{G}) = \int p_{\theta}(G | \tilde{G}; z) p_{\theta}(z | \tilde{G}) \, dz,
\]
where \( p_\theta(G \mid \tilde{G}, z) \) is the likelihood of the full graph, \( p_\theta(z \mid \tilde{G}) \) is the prior, and \( \theta \) are the learnable generative parameters. The likelihood is given by

\[
p_\theta(G \mid \tilde{G}, z) = \prod_{i=1}^{N} p_\theta(p_i \mid \tilde{G}, z_i), \quad \text{with} \quad p_\theta(p_i \mid \tilde{G}, z_i) = \mathcal{N}(p_i \mid \mu_i, \Sigma),
\]

(3)

where \( p = \{p_i\}_{i=1}^{N} \) are the positions of all \( N \) nodes, \( z = \{z_i\}_{i=1}^{N} \) are the latent embeddings of each node, and \( \mu = \{\mu_i\}_{i=1}^{N} \) are the predicted means of the distribution of node positions. We parametrize the likelihood distribution with a GNN decoder, in other words, each node, and

\[
\text{initialized point positions set to zero. We follow the common practice of only learning the mean of}
\]

Here, we parameterize the prior as a Gaussian mixture model with \( K \) components. Each Gaussian is in turn parameterized by a mean \( \mu_k = \{\mu_{k,i}\}_{i=1}^{N} \), diagonal covariance \( \sigma_k = \{\sigma_{k,i}\}_{i=1}^{N} \), and a mixing coefficient \( \pi_k = \{\pi_{k,i}\}_{i=1}^{N} \), where \( \sum_{k=1}^{K} \pi_{k,i} = 1, \forall i = 1, ..., N \). We chose a mixture model to have an expressive prior capable of capturing the latent distribution of multiple solutions.

We parameterize the prior distribution with a multi-headed GNN encoder \( \text{GNN}_{\text{prior}}(\tilde{G}) \) that outputs parameters \( \{\mu_k, \sigma_k, \pi_k\}_{k=1}^{K} \).

The goal of learning is to maximize the marginal likelihood or evidence of the data as shown in Eq. (2). As commonly done in the variational inference literature [49], we instead maximize a tractable evidence lower bound (ELBO):

\[
\mathcal{L} = \mathbb{E}_{q_\phi(z \mid G)}[\log p(G \mid \tilde{G}, z)] - \mathbb{KL}(q_\phi(z \mid G) \| p_\theta(G \mid \tilde{G})).
\]

(5)

The inference model \( q_\phi(z \mid G) \) with learnable parameters \( \phi \) is defined as:

\[
q_\phi(z \mid G) = \prod_{i=1}^{N} q_\phi(z_i \mid G), \quad \text{with} \quad q_\phi(z_i \mid G) = \mathcal{N}(z_i \mid \mu_i, \text{diag}(\sigma^2_i)).
\]

(6)

As with the prior distribution, we parameterize the inference distribution with a multi-headed GNN encoder, \( \text{GNN}_{\text{enc}}(G) \), that outputs parameters \( \mu = \{\mu_i\}_{i=1}^{N} \) and \( \sigma = \{\sigma_i\}_{i=1}^{N} \). The inference model is an approximation of the intractable true posterior \( p(z \mid G) \). We note that the resulting ELBO objective in Eq. (5) is based on an expectation with respect to the inference distribution \( q_\phi(z \mid G) \), which itself is based on the parameters \( \phi \). Since we restrict \( q_\phi(z \mid G) \) to be a Gaussian variational approximation, we can use stochastic gradient descent (i.e., Monte Carlo gradient estimates) via the reparameterization trick [49] to optimize the lower bound with respect to parameters \( \theta \) and \( \phi \).

At test time, given a goal pose and the manipulator’s geometric information encapsulated in a partial graph \( \tilde{G} \), we can use the prior network, \( \text{GNN}_{\text{prior}} \), to encode the partial graph into a latent distribution \( p_\theta(z \mid \tilde{G}) \). During training, the distribution \( p_\theta(z \mid \tilde{G}) \) is optimized to be simultaneously near multiple encodings of valid solutions by way of the KL divergence term in Eq. (5). We can sample this multimodal distribution \( z \sim p_\theta(z \mid \tilde{G}) \) as many times as needed, and subsequently decode all of the samples with the decoder network \( \text{GNN}_{\text{dec}} \) to generate IK solutions represented as complete graphs. This procedure can be done quickly and in parallel on the GPU. At present, we do not consider joint limits, self-collisions, or obstacle avoidance—we simply sample randomly. However, these constraints can be incorporated into the distance-geometric formulation of IK [9, 34]; we return to this point in Section 6.
Table 1: Performance of GGIK on 2,000 randomly generated IK problems for five different robotic manipulators. Taking 50 samples from the learned distribution, the error statistics are presented as the mean and mean minimum and maximum error per problem, the two quartiles of the distribution, as well as the percentage of “successes,” defined as solutions with a position error lower than 1 cm and rotation error lower than 1 degree. The mean MMD score measures how different GGIK’s samples are from a uniform distribution approximated by rejection sampling with error tolerances of 8 cm and 8 degrees. Note that all solutions were produced by a single model.

4.3 E(n) Equivariant Network Architecture

In this section, we discuss the choice of architecture for networks GNN_{dec}, GNN_{enc}, and GNN_{prior}. Recall that we are interested in mapping partial graphs $G$ into full graphs $\tilde{G}$. Once trained, our model maps partial point sets to full point sets $f : \mathbb{R}^{M \times D} \rightarrow \mathbb{R}^{N \times D}$, where $f$ is a combination of networks GNN_{prior} and GNN_{dec} applied sequentially. The point positions (i.e., $p$ and $\tilde{p}$) of each node in the distance geometry problem contain underlying geometric relationships that we would like to preserve in our choice of architecture. Most importantly, the point sets are equivariant to the Euclidean group E(n) of rotations, translations, and reflections. Let $S : \mathbb{R}^{M \times D} \rightarrow \mathbb{R}^{M \times D}$ be a transformation consisting of some combination of rotations, translations and reflections on the initial partial point set $\tilde{p}$. Then, there exists an equivalent transformation $T : \mathbb{R}^{N \times D} \rightarrow \mathbb{R}^{N \times D}$ on the complete point set $p$ such that:

$$f(S(\tilde{p})) = T(f(\tilde{p})).$$

To leverage this structure or geometric prior in the data, we use E(n)-equivariant graph neural networks (EGNNs) [50] for GNN_{dec}, GNN_{enc}, and GNN_{prior}. The EGNN layer splits up the node features into an equivariant coordinate or position-based part and a non-equivariant part. We treat the positions $p$ and $\tilde{p}$ as the equivariant portion and the general features $h$ as non-equivariant. For more details about the model and a proof of the equivariance property, we refer readers to [50]. We present ablation studies on the use of the EGNN network architecture in Section 5.

5 Experiments

In this section, we (i) evaluate GGIK’s capability to learn accurate solutions and generalize across common manipulators, (ii) determine whether GGIK can be used effectively to initialize local numerical IK solvers, and (iii) investigate the importance of our choice of learning architecture.

5.1 Accuracy and Generalization of GGIK Across Manipulators

In our first experiment, we evaluate the accuracy and generalization capacity of GGIK by training a single model on a dataset comprised of a variety of manipulators featuring different structures and numbers of joints. All experiments were performed on a laptop computer with a six-core 2.20 GHz Intel i7-8750H CPU and an NVIDIA GeForce GTX 1050 Ti Mobile GPU.

We evaluate a model trained on a total of 256,000 goal poses uniformly distributed over five different commercial manipulators. The success rates in Table 1 obtained by selecting the minimum error over 32 samples drawn from the learned distribution for each goal pose, suggest that this approach is feasible for directly generating solutions in a variety practical applications. As a benchmark, we trained a network on 100,000 UR10 poses using the distal teaching (DT) method of [1]. In spite of the fact that it is designed explicitly for the UR10 and saw roughly twice as many UR10 samples as our GGIK model, the DT network was only able to achieve a mean position error of 35 mm and a mean rotation error of 16 degrees. This performance is consistent with the extensive experimental results in [1], which demonstrate the strengths and shortcomings of traditional machine learning.
techniques for IK. Moreover, the position and orientation error percentiles indicate that the majority of sampled configurations correspond to end-effector poses in close proximity to the goal pose. Consequently, samples from the learned distributions such as those shown in Fig. 3 can be refined to arbitrary accuracy with only a few iterations of a local optimizer. The maximum mean discrepancy (MMD) score [51] between GGIK’s samples and a uniform distribution computed with rejection sampling is reported for each robot as the mean over 50 goal poses with 50 sample solutions for each goal pose. The MMD attains a minimum value of zero for identical distributions; a low MMD indicates that GGIK has learned a distribution that is close to uniform over the solution set for each goal pose [5]. Interestingly, while Fig. 3 indicates that GGIK successfully captures both the continuous solution sets of the redundant robots and the discrete solution sets characteristic of the 6-DOF Schunk LWA4P and UR10, the MMD scores for the two 6-DOF manipulators are significantly greater.

As a final experiment, we test the ability of GGIK to generalize outside of its training set. We train on a set of 480,000 randomly generated manipulators (instances) that have similar kinematic structures to the Kuka, lwa4d and lwa4p and test on the actual robots, whose exact structures are not included in the training dataset. Training involves randomly sampling with link lengths that vary by ±40% relative to the ‘actual’ robots. We present the results in Table 4, where each line in the table lists averages from 2000 problem. We follow the same procedure used in the experiment presented in Table 1. We note that the model is able to generalize reasonably well, and believe that the GGIK framework holds promise for even better generalization. Determining how to systematically perform randomization on the robot structure may lead to a promising method for training such models.

5.2 Initializing a Local Numerical IK Solver with GGIK

GGIK learns a sampling distribution capable of producing multiple approximate solutions in parallel, which may be used as initializations for optimization-based methods. Table 2 shows the results of repeating the experiment in Section 5.1 using an IK solver based on the SLSQP algorithm implemented in the scipy.optimize package [52], setting a maximum of 100 iterations and keeping other termination criteria at their default values. We compare the solver’s accuracy and number of iterations required before convergence when initialized with 32 random configurations per problem and 32 samples from our learned distribution. We average the results over all problems and all robots. While both approaches achieve a high degree of success and accuracy on these unconstrained problems, the results clearly show that using our model to initialize the optimization produces better overall performance. Specifically, the mean number of iterations required compared to random initializations is almost three times lower, and the accuracy of the solutions is notably higher as well. Our model could be used as a fallback approach for difficult or highly constrained instances of IK, or as a general initializer ensuring accurate final results.

5.3 Ablation Study on the Equivariant Network Architecture

We conduct an ablation experiment to evaluate the importance of capturing the underlying $E(n)$ equivariance of the distance geometry problem (Problem 3.2) in our learning architecture. We compare the use of the EGNN network [50] to four common and popular GNN layers that are not $E(n)$ equivariant: GRAPHsage [53], GAT [54], GCN [55] and MPNN [56]. We match the number of parameters for each GNN architecture as closely as possible and keep all other experimental parameters fixed. Our dataset is the same one used in Section 5.1, however the results are averaged over all manipulators as shown in Table 3. Out of the five different architectures that we compare, only the EGNN and MPNN output point sets that can be successfully mapped to valid joint configurations. Point sets that are too far from those representing a valid joint configuration result in
| Model Name | Err. Pos. [mm] mean | Err. Pos. [mm] min | Err. Pos. [mm] max | Q1 | Q3 | Err. Rot. [deg] mean | Err. Rot. [deg] min | Err. Rot. [deg] max | Q1 | Q3 | Test ELBO | Success [%] |
|------------|---------------------|-------------------|-------------------|----|----|----------------------|-------------------|-------------------|----|----|-----------|-------------|
| EGNN       | 18.4                | 5.1               | 85.8              | 10.9 | 22.5 | 1.7                  | 0.5               | 1.0               | 2.0 | 10.1 | -3.8      | 96.3        |
| MPNN       | 143.2               | 62.9              | 273.7             | 113.1 | 169.1 | 17.7                  | 5.3               | 13.6              | 21.6 | 34.1 | -8.3      | 13.1        |
| GAT        | -                   | -                 | -                 | -   | -   | -                    | -                 | -                 | -   | -   | -12.41    | 0.0         |
| GCN        | -                   | -                 | -                 | -   | -   | -                    | -                 | -                 | -   | -   | -12.42    | 0.0         |
| GRAPHsage  | -                   | -                 | -                 | -   | -   | -                    | -                 | -                 | -   | -   | -10.5     | 0.0         |

Table 3: Comparison of different network architectures. EGNN outperforms existing architectures that are not equivariant in terms of overall accuracy and test ELBO.

The configuration reconstruction procedure diverging. The equivariant EGNN model outperforms all other models in terms of the ELBO value attained on a held-out test set from our original training data. Our ablation results emphasize the importance of choosing a learning architecture that properly captures the representation utilized in the distance-geometric IK problem formulation.

### 6 Limitations and Future Work

While our proposed architecture demonstrates a capacity for generalization and to produce diverse solutions, generated solutions may require post-processing by local optimization methods in certain applications in order to adhere to constraints more tightly or to have stricter accuracies. We have demonstrated generalization by training with randomly generated but kinematically-similar to a class of existing real manipulators, and then testing on the actual existing real manipulators that were unseen during training. As interesting future work, we would like to investigate the type of data required to train GGIK in order to achieve better generalization. A potential approach would be to provide randomly generated manipulators of multiple kinematic structures. We would also like to learn constrained distributions of robot configurations that account for obstacles in the task space and for self-collisions; obstacles can be easily incorporated in the distance-geometric representation of IK [29, 34]. Learning an obstacle- and collision-aware distribution would yield a solver that implements collision avoidance by way of message passing between manipulator and obstacle nodes.

| Robot  | Err. Pos. [mm] mean | Err. Pos. [mm] min | Err. Pos. [mm] max | Q1 | Q3 | Err. Rot. [deg] mean | Err. Rot. [deg] min | Err. Rot. [deg] max | Q1 | Q3 | Success [%] |
|--------|---------------------|-------------------|-------------------|----|----|----------------------|-------------------|-------------------|----|----|-------------|
| kuka   | 27.3                | 7.2               | 124.5             | 15.4 | 29.8 | 2.5                  | 0.5               | 11.7              | 1.4 | 2.8 | 77.2        |
| lwa4d  | 134.7               | 69.9              | 275.0             | 106.9 | 151.2 | 18.1                  | 7.7               | 42.6              | 13.1 | 21.2 | 1.8         |
| lwa4p  | 101.4               | 70.4              | 140.5             | 87.0 | 114.3 | 16.8                  | 4.6               | 40.6              | 10.8 | 21.1 | 3.8         |

Table 4: Performance of GGIK on manipulators not seen during training. We train on randomly generated manipulators that have similar kinematic structures to the Kuka, lwa4d and lwa4p and test on the actual robots, which were not seen in the dataset. Taking 32 samples from the learned distribution, the error statistics are presented as the mean and mean minimum and maximum error per problem, the two quartiles of the distribution, as well as the percentage of “successes,” defined as solutions with a position error lower than 1 cm and rotation error lower than 1 degree.
7 Conclusion

We have presented GGIK, a generative graphical IK solver that is able to produce multiple diverse and accurate solutions in parallel across many different manipulator types. This capability is achieved through a distance-geometric representation of the IK problem in concert with GNNs. The accuracy of the generated solutions points to the potential of GGIK both as an approximate standalone solver and as an initialization method for local approaches. To our knowledge, this is the first approach that allows the generation of multiple solutions for multiple different robots using only a single model. Importantly, because GGIK is fully differentiable, it can be incorporated as a flexible IK solver as part of an end-to-end learning-based robotic manipulation framework.

GGIK provides a framework for and lays down some groundwork towards learned general IK – a universal initializer or solver that can provide multiple diverse solutions and can be used with any manipulators.
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Appendix

Additional Timing Experiment

We studied the scaling of the computation time as a function of the amount of samples or seeds generated by GGIK. Batch requests can take advantage of the GPU architecture and yield very low per-solution solve times when amortized across larger batches. This would be used, for example, in sampling-based motion planning and elsewhere.

![Computation Time vs Sample Size](image)

Figure 4: We plot the time taken in seconds, on the $y$-axis, as a function of the number of samples or seeds (forward passes) generated by GGIK, on the $x$-axis. We note that it takes approximately 0.01 seconds, or 10 milliseconds, to generate about 10 samples, and approximately 0.08 seconds, or 80 milliseconds, to generate 1,000 samples (i.e., $100 \times$ more samples for roughly $8 \times$ more computation time, or $0.08 \times 10^{-5}$ seconds, per sample). Error bars show one standard deviation.

Practical Training Advice

In this section, we provide some brief, practical advice for training GGIK, based on our experience. By far, the most important parameter for training was the choice of GNN architecture. Picking a network architecture that captures the underlying geometry and equivariance of the problem improved the training by a large margin as shown by Table 3 in our paper. In order to increase the accuracy of our models, we found that scheduling the learning rate when the training loss stagnated was very useful. We empirically observed that increasing the number of layers in our GNNs up to five improved the overall performance. There was very little performance improvement beyond five layers. Finally, we found that using a mixture model for the class distribution of the prior encoder also lead to better modelling results. We hypothesize that a more expressive prior distribution can better fit multiple encoded IK solutions when conditioned on a single goal pose.

Additional Experiment with the Panda Manipulator Only

| Robot | mean | min | max | $Q_1$ | $Q_3$ | mean | min | max | $Q_1$ | $Q_3$ | Success [%] |
|-------|------|-----|-----|-------|-------|------|-----|-----|-------|-------|-------------|
| panda | 22.0 | 2.7 | 135.0 | 8.3 | 23.3 | 2.2 | 0.2 | 13.5 | 0.9 | 2.4 | 99.2 |

Table 5: Error analysis for 2,000 samples generated with a model solely trained on the Panda robot.
We ran an additional experiment to determine the performance of GGIK when trained on data from the Panda manipulator alone. This experiment also permits a preliminary, rough comparison of GGIK with the IKFlow algorithm [5].

The Panda has an interesting, asymmetric structure that differs from the symmetric structure of other robot models used for training. We believe this structure may present a more difficult learning problem, due to an inherent property of the distance-based robot representation in [9], where asymmetric linkages produce ambiguities in the solution space. More specifically, even though our model avoids these ambiguities with a position-based loss, the Panda robot remains the only one in our training set with such an asymmetric structure, and is therefore underrepresented.

To examine this, we trained a model on the Panda arm only, using our standard procedure with 256K random training samples (robot configurations). The results, presented in Table 5, shows that training on the Panda by itself improves Panda-specific performance (in terms of error reduction) by some margin, relative to the results in Table 1 of the main manuscript. This would make sense since our loss is based on positions and not on distances, and the GGIK network should be able learn to disambiguate reflections in the representation by training only on points that represent feasible configurations. Indeed, the Panda-only training reduces the average errors to be much closer to those for other robots in Table 1 of the main paper.

We highlight two important, related notes. First, existing work [34] explicitly facilitates use of manipulators with structures like those of the Panda (i.e., asymmetries); our overall network design could potentially support modifications that would help to solve IK problems for these manipulators. Second, the reduction in error with the Panda-only model leads us to believe that the performance could be further improved by diversifying and enlarging the training dataset to include robots with randomized structures. The required network modifications, as well as the introduction of randomized robot models in a systematic manner during training, are both intricate problems that we leave for a future, extended treatment.