Abstract: Multi-objective high-dimensional motion optimization problems are ubiquitous in robotics and highly benefit from informative gradients. To this end, we require all cost functions to be differentiable. We propose learning task-space, data-driven cost functions as diffusion models. Diffusion models represent expressive multimodal distributions and exhibit proper gradients over the entire space. We exploit these properties for motion optimization by integrating the learned cost functions with other potentially learned or hand-tuned costs in a single objective function, and optimize all of them jointly by gradient descent. We showcase the benefits of the joint optimization in a set of complex grasp and motion planning problems and compare against hierarchical approaches that decouple the grasp selection from the motion optimization. Videos and code at: https://sites.google.com/view/se3dif

Keywords: diffusion models, generative models, grasping, trajectory optimization, energy-based models

1 Introduction

Autonomous robot manipulation tasks usually involve complex actions requiring a set of sequential or recurring subtasks to be achieved while satisfying certain constraints, thus, casting robot manipulation into a multi-objective motion optimization problem [1, 2, 3]. Let us consider the pick-and-place task in Fig. 1, for which the motion optimization should consider the possible set of grasping and placing poses, the trajectories’ smoothness, collision avoidance with the environment, and the robot’s joint limits. While some objectives are easy to model (e.g., joint limits, trajectory smoothness), others (e.g., collision avoidance, grasp pose distribution) are more expensive to model, and therefore commonly approximated by learning-based approaches [4, 5, 6, 7, 8].

Data-driven models are usually integrated into motion optimization either as sampling functions (explicit generators) [6, 9], or cost functions (scalar fields) [10, 4]. When facing multi-objective optimization scenarios, the explicit generators do not allow a direct composition with other objectives, thereby requiring two, or even more separate optimization phases [11]. Contrarily, learned scalar fields represent task-specific costs that can be combined with other learned or heuristic cost functions to form a single objective function. This allows for one single joint optimization. Yet, these cost functions are often learned with objectives like cross-entropy [6, 12] or contrastive divergence [13, 10] that try to create hard discriminating regions in the modeled data, leading to large plateaus in the learned field with zero or noisy slope regions [14, 15], thereby unsuitable for pure gradient-based optimization. Thus, it is a common strategy to rely on task-specific samplers that first generate samples close to low cost regions before optimizing [6, 12].

In this work, we instead propose to learn smooth data-driven cost functions by drawing inspiration from state-of-the-art diffusion generative models [16]. With smoothness we refer to the cost function exposing informative gradients in the entire space. We propose learning these smooth cost functions in the SE(3) robot’s workspace, thus defining task-specific costs. In particular, we learn diffusion models for 6D grasp pose generation given the Acronym dataset [17]. The resulting models allow to move randomly initialized samples to the low-cost regions by evolving a gradient-based inverse diffusion process [18] (cf. Fig. 2).

Additionally, we propose a formulation for framing robot motion generation as an inverse dif-
fusion, by combining our learned diffusion model for 6D grasp pose generation with other smooth costs (trajectory smoothness cost, collision avoidance cost, etc.). All the objectives together form one single, smooth cost function enabling to recover good trajectories through gradient-based inverse diffusion. We therefore optimize all the trajectories’ waypoints through running an inverse diffusion process on the trajectory level. This allows to seamlessly acquire task-specific trajectories in challenging environments (Fig. 1).

To summarize our contributions, (1) we propose learning smooth cost functions in SE(3) as diffusion models. As SE(3) is a non-Euclidean space, we show a practical approach to adapt the training and sampling processes of diffusion models; (2) we provide a single gradient-based optimization framework for jointly resolving grasp and motion generation, which allows effective integration of additional costs with our smooth cost function over grasps. The framework enables to resolve complicated multi-objective trajectory optimization problems that might not only include optimization w.r.t. the object-grasp configuration but also conditioning on a desired placing pose.

2 Background

Diffusion Models. Unlike common deep generative models (Variational Autoencoders (VAE), Generative Adversarial Networks) that explicitly generate a sample from a noise signal, diffusion models learn to generate new samples by smoothly moving noisy random samples towards the data distribution \( \rho_D(x) \) by denoising [19, 16]. A common approach to train diffusion models is by Denoising Score Matching (DSM) [20]. To apply DSM [19, 21], we first perturb the data distribution \( \rho_D(x) \) with Gaussian noise on \( L \) noise scales \( \mathcal{N}(0, \sigma_k I) \) with \( \sigma_1 < \sigma_2 < \cdots < \sigma_L \), to obtain a noise perturbed distribution \( q_{\sigma_k}(\hat{x}) = \int x \mathcal{N}(x|\hat{x}, \sigma_k I) \rho_D(x)dx \). To sample from the perturbed distribution, \( q_{\sigma_k}(\hat{x}) \) we first sample from the data distribution \( x \sim \rho_D(x) \) and then add white noise \( \hat{x} = x + \epsilon \) with \( \epsilon \sim \mathcal{N}(0, \sigma_k I) \). Next, we estimate the score function of each noise perturbed distribution \( \nabla_x \mathcal{N}(x|\hat{x}, \sigma_k^2 I) \) by training a noise-conditioned Energy Based Models (EBM) \( E_\theta(x, k) \), by score matching \( \nabla_x E(x, k) \approx -\nabla_x \log q_{\sigma_k}(x) \) for all \( k = 1, \ldots, L \). The training objective equates to

\[
L_{\text{dsm}} = \frac{1}{L} \sum_{k=0}^{L} \lambda(k) \mathbb{E}_{x \sim \rho_D(x), \hat{x} \sim \mathcal{N}(x, \sigma_k I)} \left[ \left\| \nabla_{\hat{x}} E_\theta(\hat{x}, k) + \nabla_{\hat{x}} \log \mathcal{N}(\hat{x}|x, \sigma_k^2 I) \right\| \right],
\]

with \( \lambda(k) > 0 \). To generate samples from the trained model, we apply Annealed Langevin Markov Chain Monte Carlo (MCMC) [22]. We first draw an initial set of samples from a distribution \( x_L \sim \rho_L(x) \) and then, simulate an inverse Langevin diffusion process for \( L \) steps, from \( k = L \) to \( k = 1 \)

\[
x_{k-1} = x_k - \frac{\alpha_k}{2} \nabla_{x_k} E_\theta(x_k, k) + \alpha_k \epsilon, \ \epsilon \sim \mathcal{N}(0, I),
\]

with \( \alpha_k > 0 \) a step dependent coefficient. Overall, DSM (1) learns models whose gradients point towards the samples of the training dataset [18].

SE(3) Lie group. The SE(3) Lie group is prevalent in robotics. A point \( H = \begin{bmatrix} R & t \end{bmatrix} \in \text{SE}(3) \) represents the full pose (position and orientation) of an object or robot link with \( R \in \text{SO}(3) \) the rotation matrix and \( t \in \mathbb{R}^3 \) the 3D position. A Lie group encompasses the concepts of group and smooth manifold in a unique body. Lie groups are smooth manifolds whose elements have to fulfill certain constraints. Moving along the constrained manifold is achieved by selecting any velocity withing the space tangent to the manifold at \( H \) (i.e., the so-called tangent space). The tangent space

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1 In [19, 21] the score function is trained directly, rather than the energy function \( E_\theta \). In our case, we are interested in the energy, as we can use it as a cost function.
at the identity is called Lie algebra and noted se(3). The Lie algebra has a non-trivial structure, but it is isomorphic to the vector space $\mathbb{R}^6$ in which we can apply linear algebra. As in [23], we work in the vector space $\mathbb{R}^6$ instead of the Lie algebra $\text{se}(3)$. We can move the elements between the Lie group and the vector space with the logarithmic and exponential maps, $\text{Logmap} : \text{SE}(3) \rightarrow \mathbb{R}^6$ and $\text{Expmap} : \mathbb{R}^6 \rightarrow \text{SE}(3)$ respectively [23]. A Gaussian distribution on Lie groups can be defined as

$$q(H|\mu, \Sigma) \propto \exp\left(-0.5 \| \text{Logmap}(H^{-1}\mu) \|_{\Sigma^{-1}}^2 \right),$$

with $H_{\mu} \in \text{SE}(3)$ the mean and $\Sigma \in \mathbb{R}^{6 \times 6}$ the covariance matrix [24]. This special form is required as the distance between two Lie group elements is not represented in Euclidean space.

Following the notation of [23], given a function $f : \text{SE}(3) \rightarrow \mathbb{R}^n$, the Jacobian w.r.t. a SE(3) element, $J = Df(H)/DH \in \mathbb{R}^{n \times 6}$ is a matrix of shape $6 \times n$. As shown in App. A.1 (13), the derivatives w.r.t. SE(3) elements are obtained through investigating the change in the functions outputs w.r.t. infinitesimal variations expressed in tangent spaces. For an extended introduction to Lie group theory please see App. A.

3 SE(3)-Diffusion Fields

In this work, we propose a practical extension of diffusion models to the Lie group $\text{SE}(3)$ [23], as it is a crucial space for robot manipulation. The $\text{SE}(3)$ space is not Euclidean, hence, multiple design choices need to be considered for adapting Euclidean diffusion models. In the following, we first explain the required modifications (Sec. 3.1), then, propose a neural network architecture for learning $\text{SE}(3)$ diffusion models (Sec. 3.2). Finally, we show how to integrate the learned diffusion models into a multi-objective motion optimization problem (Sec. 3.3).

3.1 From Euclidean diffusion to diffusion in SE(3)

We call $\text{SE}(3)$-DiffusionFields (SE(3)-DiF) a scalar field that outputs a scalar value $e \in \mathbb{R}$ for an arbitrary query point $H \in \text{SE}(3)$

$$e = E_{\theta}(H, k),$$

with scalar conditioning variable $k$ determining the current noise scale [19].

**Denoising Score Matching in SE(3).** Similar to the Euclidean space version (cf. Sec. 2), DSM is applied in two phases. We first generate a perturbed data point in SE(3), i.e., sample from the Gaussian on Lie groups (3), $H \sim q(H|H, \sigma_k I)$ with mean $H \in \rho_D(H)$ and standard deviation $\sigma_k$ for noise scale $k$. Practically, we sample from this distribution using a white noise vector $\epsilon \in \mathbb{R}^6$,

$$\tilde{H} = \text{HExpmap}(\epsilon), \; \epsilon \sim \mathcal{N}(0, \sigma_k^2 I).$$

Following the idea of DSM, the model is trained to match the score of the perturbed training data distribution. Thus, DSM in SE(3) requires computing the gradients of the model and the perturbed distribution w.r.t. a Lie group element. Hence, the new DSM loss function on Lie groups equates to

$$\mathcal{L}_{\text{ds}} = \frac{1}{L} \sum_{k=0}^{L} \lambda(k) E_{H \sim \rho_D(H), H \sim q(H|H, \sigma_k I)} \left[ \frac{DE_{\theta}(\tilde{H}, k)}{D\tilde{H}} + \frac{D \log q(\tilde{H}|H, \sigma_k I)}{D\tilde{H}} \right].$$

We add additional details on the computation of the derivatives in App. A.1. In practice, we follow the implementations of [25] and compute an approximation of the derivatives (cf. App. A.1.2). We add a comparison w.r.t. the mathematically sound approach in App. D.5.

**Sampling with Langevin MCMC in SE(3).** Evolving the inverse Langevin diffusion process for
SE(3) elements (cf. Fig. 2 for visualization) requires adapting the previously presented version (2). In particular, we have to ensure staying on the manifold throughout the inverse diffusion process. Thus, the equation for inverse diffusion in SE(3) is given by

\[
H_{k-1} = \text{Expmap} \left( -\frac{\alpha_k^2}{2} \frac{DE_{\theta}(H_k, k)}{DH_k} + \alpha_k \epsilon \right) H_k, \epsilon \sim \mathcal{N}(0, I),
\]

with the step dependent coefficient \( \alpha_k > 0 \) and \( \epsilon \in \mathbb{R}^6 \) a white noise vector. Note that the derivative \( DE_{\theta}(H_k, k)/DH_k \) outputs a \( \mathbb{R}^6 \) vector (see App. A.1 for additional details).

### 3.2 Architecture & training of SE(3)-GraspDiffusionFields

Even though SE(3)-DiF can represent any data-driven cost in SE(3), in this work, we focus on cost functions that capture 6D grasp pose distributions. To this end, our cost function should be conditioned on information regarding the object we aim to grasp (object pose and shape). In the main paper, we do not investigate the perception aspect of encoding point clouds into object pose and shape [6, 26]. Our implementation assumes that we can rely on state-of-the-art object pose detection and segmentation. We therefore learn a latent feature representation for encoding every object shape [6, 26]. Our implementation assumes that we can rely on state-of-the-art object pose detection and segmentation. We therefore learn a latent feature representation for encoding every object shape [6, 26]. Our implementation assumes that we can rely on state-of-the-art object pose detection and segmentation. We therefore learn a latent feature representation for encoding every object shape [6, 26]. Our implementation assumes that we can rely on state-of-the-art object pose detection and segmentation. We therefore learn a latent feature representation for encoding every object shape [6, 26]. Our implementation assumes that we can rely on state-of-the-art object pose detection and segmentation. We therefore learn a latent feature representation for encoding every object shape [6, 26].

Learning implicit functions [27, 28] that represent the geometric properties of an object can enhance the quality of grasp pose generation models [26, 29]. Following the same intuition, we propose to jointly learn the objects’ Signed Distance Field (SDF) and the grasp diffusion model. Our proposed architecture for SE(3)-DiF is illustrated in Fig. 3. It consists of three parts for mapping from object shape and grasp pose to grasp quality, i.e., energy: (I) the grasp pose encoder, (II) the feature encoder and, (III) the decoder function. The grasp pose encoder receives as input the SE(3) grasp pose \( H^g_w \). The grasp pose is used to transform a fixed set of 3D-points around the grasp’s center, i.e., the gripper \((x_g \in \mathbb{R}^N \times 3)\), into the world frame by \( x_w = H^w_g x_g \) \((x_w \in \mathbb{R}^N \times 3)\). We thereby express the pose through the points’ positions, similar to [29]. Given the object’s index \( m \), we retrieve its shape code \( z_m \in \mathbb{R}^3 \) and pose \( H^m_w \in SE(3) \). The pose allows to transform the points representing the grasp into the object’s local frame, \( x_{om} = H^m_w x_w \). Given that everything is now conveniently centered around the object, we apply the feature encoding network \( F \) which is also conditioned on \( z_m \) and \( k \in \mathbb{R}^+ \) to inform about the object type and noise level, respectively [16]. The encoding network outputs both the SDF predictions for the query points, i.e., \( sdf_m(x_{om}) \in \mathbb{R}^{N \times 1} \), and a set of additional features \( \psi \in \mathbb{R}^{N \times \psi} \). Thus, the feature encoder’s output is of size \( N \times (1 + \psi) \). Next, the object-centric features are flattened and passed through the decoder \( D \) to obtain the scalar energy value \( \epsilon \) representing the grasp’s quality. During training, we jointly learn the objects’ latent codes \( z_m \) and the parameters \( \theta \) of the feature encoder \( F \) and decoder \( D \).

The training objective function, subject to minimization, is designed to emphasize the joint learning of grasp diffusion by matching the denoising score \( \mathcal{L}_{\text{ldm}} \), and the object’s SDF \( \mathcal{L}_{\text{ldf}} \) (as in [27]) for instilling geometric reasoning and regularization,

\[
\mathcal{L} = \mathbb{E}_{(o_m, H^w_g)} \sim \rho_{\text{grasp}} \left[ \mathcal{L}_{\text{ldm}}(H^m_w, H^w_g, z_m, \theta) \right] + \mathbb{E}_{(x_o, o_m)} \sim \rho_{\text{df}} \left[ \mathcal{L}_{\text{ldf}}(x_o, sdf_m, z_m, \theta) \right]
\]

with \( x_o \in \mathbb{R}^3 \) a randomly sampled point in object’s \( o_m \) frame, \( sdf_m \) the object’s groundtruth SDF, the object’s shape code \( z_m \), and \( H^w_g \) & \( H^m_w \) parameterizing an SE(3) grasp pose given the gripper points \( x_g \). During training we assume \( H^m_w \) to be identity. We provide pseudocode for the complete training procedure in App. B.1, and the details of the architecture in App. C.

### 3.3 Grasp and motion generation with diffusion models

Given a trajectory \( \tau : \{q_t\}_{t=1}^T \), consisting of \( T \) waypoints, with \( q_t \in \mathbb{R}^d \) describing the robot’s joint positions at time instant \( t \), in motion optimization, we aim to find the minimum cost trajectory

\[
\tau^* = \arg \min_{\tau} J(\tau) = \arg \min_{\tau} \sum_j \omega_j c_j(\tau),
\]

defining objective function \( J \) as a weighted sum of costs \( c_j \), with weights \( \omega_j > 0 \). Herein, we integrate the learned SE(3)-DiF for grasp generation as one term of the cost function. It is thus combined with other heuristic costs representing, for instance, collision avoidance or trajectory smoothness. Optimizing over the whole set of costs enables obtaining optimal trajectories jointly taking into account grasping, as well as motion related objectives. This differs from classic motion planning approaches in which the grasp pose sampling and the trajectory planning are treated separately [30], by
MCMC over a trained classifier for pose refinement. In this experiment, we assume the object’s Net generates grasps by first sampling from a decoder of a trained VAE and subsequently running We compare against three baselines. All baselines are variations of 6-dof GraspNet [6]. Grasp-diffusion process ((7), pseudocode in App. B.2), using (19) as initial sampling distribution. To eliminate any other influence, we only consider the gripper and assume that we can set it to any arbitrary pose. We generate the 6D grasp poses from SE(3)-DiF by an inverse diffusion process for sufficient steps, the particles at $\tau_k$ that evolves a set of random initial particles drawn from a distribution $p_0$. Given the resulting points $x_o$ and the object’s shape code $z$ we apply the feature encoder $F_\theta$ (II) to obtain a object and grasp-related features (sdf, $\psi$) $\in \mathbb{R}^{N \times (\psi+1)}$. Finally, we flatten the features and compute the energy $e$ through the decoder $D_\theta$ (III).

first sampling the grasp pose and then searching for a trajectory that satisfies the selected grasp pose. Given that the learned function is in SE(3) while the optimization is w.r.t. the robot’s joint space, we redefine the cost as $c(q, k) = E_\theta(\phi_{ee}(q, k))$, with the forward kinematics $\phi_{ee} : \mathbb{R}^{d_q} \rightarrow \text{SE}(3)$ mapping from robot configuration to the robot’s end-effectors task space. Intuitively, this cost function provides low cost to those robot configurations that lead to good grasps. To obtain minimum cost trajectories, we frame the motion generation problem as a inverse diffusion process. The desired target distribution is now defined as $q(\tau|k) \triangleq \exp(-J(\tau, k))$ using a planning-as-inference view [31, 32, 33]. This allows us to set an inverse Langevin diffusion process that evolves a set of random initial particles drawn from a distribution $\tau_L \sim p_L(\tau)$ towards the target distribution $q(\tau|k)$

$$\tau_{k-1} = \tau_k + 0.5 \alpha_k \nabla_{\tau_k} \log q(\tau|k) + \alpha_k \epsilon, \epsilon \sim \mathcal{N}(0, I),$$

with step dependent coefficient $\alpha_k > 0$, the noise level moving from from $k = L$ to $k = 1$, and one particle corresponding to an entire trajectory. If we evolve the particles by this reverse diffusion process for sufficient steps, the particles at $k = 1$, $\tau_1$ can be considered as particles sampled from $q(\tau|k = 1)$. To finally obtain the optimal trajectory, we evaluate the samples on $J(\tau, 1)$ and pick the one with the lowest cost. See also the pseudocode in App. B.3. A similar approach has been recently proposed in [34].

4 Experimental evaluation

We train SE(3)-DiF as a 6D grasp pose generative model using the Acronym dataset [17]. This simulation-based dataset contains labelled 6D grasp poses (successful/unsuccesful grasp) for a variety of objects from the ShapeNet repository [35]. In particular, as we want to learn the distribution of good grasping poses, we focus on the collection of successful grasp poses for 90 different mugs (approximately 90K 6D grasp poses). We obtain the mugs’ meshes from the ShapeNet repository [35] and train the model as described in Sec. 3.2. The evaluation is divided in two parts. In the first part, we evaluate our trained model for 6D grasp pose generation (Sec. 4.1) and investigate the generated grasps on quality and diversity. In the second part, we evaluate the quality of our trained model when used as an additional cost term for robot grasp configuration or motion optimization problems (Sec. 4.2). Finally, we add real robot experiments in App. D.6. We perform all our simulated experiments in Nvidia Isaac Sim [36].

4.1 Evaluation of 6D grasp pose generation

We want to validate that our SE(3)-DiF model generates diverse, high-quality grasps by evaluating the success rate, and the Earth Mover Distance (EMD) between the generated grasps and the training data distribution. The EMD measures the divergence between two empirical probability distributions [37]. To eliminate any other influence, we only consider the gripper and assume that we can set it to any arbitrary pose. We generate the 6D grasp poses from SE(3)-DiF by an inverse diffusion process ((7), pseudocode in App. B.2), using (19) as initial sampling distribution. We compare against three baselines. All baselines are variations of 6-dof GraspNet [6]. GraspNet generates grasps by first sampling from a decoder of a trained VAE and subsequently running MCMC over a trained classifier for pose refinement. In this experiment, we assume the object’s
Figure 4: 6D grasp pose generation experiment with \( n_s = 200 \) initial samples. Left: Success rate evaluation. Center: EMD evaluation metrics (lower is better). Right: A visual example of 10 non-cherry picked grasps sampled with Langevin MCMC on SE(3)-DiF as presented in (7).

For ensuring a fair comparison, we replace GraspNet’s point cloud encoder with a DeepSDF autodecoder [27], that gets as input the object’s pose and id. The resulting three baselines are: 1) sampling as proposed in GraspNet (VAE+ refinement), 2) sampling from the VAE (without any further refinement) and, 3) solely running MCMC over the classifier starting from random initial pose.

We present the results in Fig. 4. In terms of success rate, SE(3)-DiF outperforms VAE + classifier slightly (especially yielding lower variance), and VAE / classifier on their own significantly. The VAE alone generates noisy grasp poses that are often in collision with the mug. In the case of classifier only, the success rate is low. We hypothesize that this might be related with the classifier’s gradient, as specifically in regions far from good samples, the field has a large plateau with close to zero slopes [14]. This leads to not being able to improve the initial samples. Considering grasp diversity, i.e., EMD metric (lower is better), SE(3)-DiF outperforms all baselines significantly. A reason for the difference, might be that VAE + classifier overfits to specific overrepresented modes of the data distribution. In contrast, SE(3)-DiF’s samples capture the data distribution more properly. We, therefore, conclude that SE(3)-DiF is indeed generating high-quality and diverse grasp poses.

We add an extended presentation of the experiment in App. D.1.

4.2 Evaluating robot grasp configuration generation and motion optimization

In the following, we evaluate the flexibility of our 6D grasp generative model SE(3)-DiF as a cost term in multi-objective optimization problems. All scenarios include the whole Franka Panda arm and the mugs placed on a table. We consider two different problems: (a) generating grasps by optimizing for the robot’s joint configuration and (b) joint grasp and motion optimization, i.e., considering whole trajectories. We also add real robot evaluations in App. D.6 and on the website.

**Robot grasp configuration generation.** We consider the problem of finding robot joint configurations resulting in successful and feasible grasps. This is a multi-objective optimization as successful solutions require compatibility of the desired grasp pose and the robot’s workspace while avoiding table collisions. We propose solving the problem as a single optimization problem as presented in Sec. 3.3. We exploit differentiable forward kinematics to map a robot configuration to the end effector’s space (SE(3)) and evaluate grasp quality using SE(3)-DiF. We add additional cost terms and optimize the robot’s joint configuration \( q \) over the total set of costs (more details in App. D.2). The initial samples are sampled from a uniform distribution bounded by the joint limits’.

As baselines we consider two methods. The first (joint opt - classifier) applies our proposed joint optimization scheme, yet replacing SE(3)-DiF with the trained classifier from Sec. 4.1. The second (sample + opt), considers a separate two-stage optimization, in which we first sample SE(3) grasp poses using SE(3)-DiF as in the previous experiment. This sampling neglects the robot’s kinematic constraints and potential table collisions. In the second step, we optimize the robot’s joint configuration to match the desired grasp poses from the first step and avoiding table collisions. Such separate, multi-stage optimization procedures have previously been proposed for handling robot grasp pose generation in very similar settings and achieve state-of-the-art performance [11, 38, 39, 40, 41].

We report averaged results across all mugs considering \( n_s = 100 \) initial samples and evaluate grasp quality by attempting to lift the mugs starting from the proposed robot configuration. The results in Table 1 reveal that across all experiments, our proposed joint optimization procedure results in the highest success rates \( s_\Omega \) and \( s_1 \), i.e., considering evaluating all particles, and only the best one, respectively. In line with the previous results, the learned classifier’s energy landscape is not suitable for gradient-based optimization and hence results in lowest successes. The separate optimization (sample + opt) performs substantially better, but still worse compared to our proposed
Figure 5: Grasp and Motion Optimization. Left: Success rate w.r.t. the number of initialized particles for a set of different tasks. Center: A visualization of the picking with occlusion task (pick). Right: A visualization of the pick and reorient task.

Joint optimization with SE(3)-DiF. Particularly, the experiments showcase a performance drop w.r.t. the flipped mug scenario. This underlines the major shortcoming of not being adaptive w.r.t. the current environment, i.e., sampling grasps which are simply infeasible. Contrarily, for our proposed method $s_1$ drops only slightly, and $s_1$ even remains high at 0.88. We, thus, conclude that end-end gradient-based optimization with our SE(3)-DiF model results in highly performant, reliable, and adaptive robot grasp pose generation, despite the multi-objective scenario (more details in App. D.2).

Grasp and motion optimization. We now inspect more complex tasks that require the planning of both grasp and motion on the trajectory level. We consider three tasks: picking with occlusions, picking and reorienting an object, and pick and place in shelves (see Fig. 1 & Fig. 5). Similarly to the grasp configuration problem, we propose solving it through a joint optimization (cf. Sec. 3.3, pseudocode in App. B.3) and provide all cost terms’ definitions in App. D.3. The initial trajectory samples are obtained from a Gaussian distribution with a block diagonal matrix as in [2].

We evaluate the success rate of the trajectory optimization given a different number of initial samples. As gradient-based trajectory optimization methods are inherently local optimization methods, multiple initializations might lead to better results. For the case of picking under occlusions, we again consider as baseline a hierarchical approach (sample+opt) in which we first sample an SE(3) grasp pose before running a second optimization for obtaining the robot trajectories while keeping the grasps fixed. This decoupled approach (1. plan the grasp pose, 2. path planning to the grasp) has been the standard approach in the literature [42, 43, 11].

The results in Fig. 5 display a clear benefit from the joint optimization w.r.t. the hierarchical sample+opt approach. In particular, our proposed joint optimization only requires 25 particles to match the success rate of the hierarchical approach with 800 particles. The reason for this significant gap in efficiency is that the hierarchical approach generates SE(3) grasp poses that are not feasible given the environment constraints, such as occlusions or joint limits. Yet, when optimizing jointly, we can find trajectories that satisfy all the costs by iteratively improving entire trajectories w.r.t. all objectives. Observing the results for pick-place and pick-reorient tasks, we see that our joint optimization approach results in high success rates with sufficient initial samples, and thereby demonstrate its capability to even incorporate conditions w.r.t. desired placing configurations (more in App. D.3).

4.3 Limitations

In our experiments, we focus on evaluating our diffusion model’s performance in grasp generation, besides full trajectory optimization, assuming full state knowledge. We highlight that the method we use to compute the derivatives is an approximation. It is not able to properly take the geometry of the manifold into account. Moreover, with increasing number of cost terms, it becomes more difficult to weight them. In the future, we thus consider adding automatic tuning of these hyperparameters (i.e., Bayesian Optimization) to make the method scale better. Potential sim2real discrepancies w.r.t. the real environment could potentially arise from imperfect perception, and hand-designed cost terms that may not capture well the respective task description, especially in more complex scenarios.

5 Related work

6D grasp generation. 6D grasp pose generation is solved with a myriad of methods from classifiers to explicit samplers. [38, 40, 44] sample candidate grasps and score them with learned classifiers.
[45] predicts grasping outcomes using a geometry-aware representation. Contrary to methods classifying grasps, generative models can be trained to generate grasp poses from data [6] but might require additional sample refinement. While the generator in [46] considers possible collisions in the scene, [47] proposes to learn a grasp distribution over the object’s manifold. [26] uses scene representation learning to learn grasp qualities and explicitly predict 3D rotations.

**Integrated grasp and motion planning.** Due to the interdependence of the selected grasp pose with the robot motion, multiple efforts have tried to integrate both variables into a single planning problem. In [48, 49], goal sets representing grasp poses are integrated as constraints in a motion optimization problem. In [50, 51], Rapidly-exploring Random Trees [52] is combined with a TCP attractor to bias the tree towards good grasps. [53] proposes an iterative procedure to optimize both the grasp pose and the motion. Our work differs from previous methods as we propose to set the grasp pose objective as a learned cost function in a gradient-based motion optimization problem.

**Learning cost functions.** Learned cost functions are prevalent in robotics research [54]. Particularly when it comes to constructing SDFs for motion planning [55], or using SDFs for forming optimization costs [56]. Learning implicit representations of objects can be leveraged as costs for motion optimization [57, 10] and control [58]. Highly related to our work is the field of Inverse Reinforcement Learning [59, 60, 61, 13], where the goal is to learn a cost function from demonstrations.

### 6 Conclusion

We propose SE(3)-DiffusionFields (SE(3)-DiF) for learning task-space, data-driven cost functions, aimed at enabling robotic motion generation through joint gradient-based optimization over a set of combined cost functions. At the core of SE(3)-DiFs is a diffusion model that provides informative gradients across the entire space, and thereby enables data generation through running an inverse Langevin dynamics diffusion process. Besides demonstrating that we can learn an SE(3)-DiF for generating diverse and high-quality grasp poses, we also draw a connection between motion generation and inverse diffusion, and present a framework for joint, gradient-based trajectory optimization, which we compare against a hierarchical approach with split grasp and motion optimization. Our extensive experimental evaluations reveal superior performance of the proposed method w.r.t. efficiency, adaptiveness, and success rates. In the future, we want to explore diffusion models for reactive motion control and also, explore the composition of multiple diffusion models to solve complex manipulation tasks in which multiple hard to model objectives might arise.
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A Theory on SE(3) Lie group: derivatives and distributions

The Lie group SE(3) is prevalent in robotics. A point $H \in \text{SE}(3)$ represents the full pose (position and orientation) of an object or robot link

$$H = \begin{bmatrix} R & t \\ 0 & 1 \end{bmatrix} \in \text{SE}(3)$$ (11)

with $R \in \text{SO}(3)$ the rotation matrix and $t \in \mathbb{R}^3$ the 3D position. A Lie group is both a group and a differentiable manifold (See [23] for additional details on groups). Given SE(3) is a differentiable manifold, for any point $H \in SE(3)$, there exists a tangent space centered around $H$ that is locally diffeomorphic to SE(3). The tangent space can be afterwards map to a Cartesian vector space $\mathbb{R}^6$. In particular, the tangent space at identity is known as Lie algebra and is noted by $se(3)$.

We can interact between the Lie group and the Lie algebra through the logmap and expmap functions. The logmap is a function that maps a point $H \in \text{SE}(3)$ to the Lie algebra $se(3)$, logmap : $\text{SE}(3) \rightarrow se(3)$. Inversely, the expmap moves the points $h^\wedge \in se(3)$ to the Lie group SE(3), expmap : $se(3) \rightarrow \text{SE}(3)$. Additionally, we can relate the elements in the Lie algebra $se(3)$ with the Cartesian vector space $\mathbb{R}^6$ through the hat and vee functions. The hat function $(\cdot)^\wedge : \mathbb{R}^6 \rightarrow se(3)$ maps the points in the vector space $h \in \mathbb{R}^6$ to the Lie algebra $se(3)$. Inversely, the vee function $(\cdot)\vee : se(3) \rightarrow \mathbb{R}^6$, moves the points in the Lie algebra $h^\wedge \in se(3)$ to the vector space $\mathbb{R}^6$. The vector space $\mathbb{R}^6$ is isomorphic to $se(3)$. Then, we can move any point from $se(3)$ to $\mathbb{R}^6$ and back. Nevertheless, $h \in \mathbb{R}^6$ representation is more useful in our case as we can apply Linear algebra on them. Finally, we additionally call Logmap the map from SE(3) to $\mathbb{R}^6$, Logmap = logmap$(\cdot)\vee : \text{SE}(3) \rightarrow \mathbb{R}^6$ and Expmap the map from $\mathbb{R}^6$ to SE(3). Expmap = expmap$(\cdot)^\wedge : \mathbb{R}^6 \rightarrow \text{SE}(3)$. Note that we use the upper case (Logmap, Expmap) to represent a mapping to the vector space and the lower case (logmap, expmap) to represent the mapping to the Lie algebra.

A vector field $f : \text{SE}(3) \rightarrow \mathbb{R}^6$ is a function that outputs a vector in the Cartesian vector space $\mathbb{R}^6$ for any point in SE(3). The vector’s values are dependent on a particular tangent space centered at $H \in \text{SE}(3)$. Given that there exist infinite tangent spaces (one per point in SE(3)), the value of the vectors might vary depending on the tangent space. We can transform the vectors related with one tangent space to another, with the adjoint matrix operator. The adjoint matrix operator is a linear map $h_1 = A_h h_0$, that transform a vector $h_0 \in \mathbb{R}^6$ tied with the tangent space centered at $H_0 \in \text{SE}(3)$ to the vector $h_1 \in \mathbb{R}^6$ tied with the tangent space centered at $H_1 \in \text{SE}(3)$.

A.1 Derivatives on Lie groups

To properly define derivatives on Lie groups, we are required to consider the geometry of the manifold. Given a function $f(\cdot) : \mathbb{R}^m \rightarrow \mathbb{R}^n$, the Jacobian is defined as

$$J = \frac{\partial f(x)}{\partial x} \stackrel{\text{def}}{=} \lim_{\tau \rightarrow 0} \frac{f(x + \tau) - f(x)}{\tau} \in \mathbb{R}^{n \times m},$$ (12)

with $\tau \in \mathbb{R}^m$. Nevertheless, if we aim to compute the Jacobian on the SE(3) Lie group, we are required to adapt the formulation, as we cannot directly sum $x$ and $\tau$. Given a function $f(\cdot) : \mathcal{M} \rightarrow \mathcal{N}$ from the manifold $\mathcal{M}$ to the manifold $\mathcal{N}$, the Jacobian is defined as

$$\frac{Df(X)}{DX} \stackrel{\text{def}}{=} \lim_{\tau \rightarrow 0} \frac{f(\tau \odot X) \ominus f(X)}{\tau} = \lim_{\tau \rightarrow 0} \frac{\logmap(f(X)^{-1}f(\expmap(\tau)X))}{\tau} \in \mathbb{R}^{m \times n},$$ (13)

where $m$ is the dimension of the manifold $\mathcal{M}$ and $n$, the dimension of the manifold $\mathcal{N}$, $X \in \mathcal{M}$ is an element in $\mathcal{M}$ and the output $f(X) \in \mathcal{N}$ an element in $\mathcal{N}$. The plus $\oplus$ and minus $\ominus$ operators must be selected appropriately; $\oplus$ for the domain $\mathcal{M}$ and $\ominus$ for the codomain $\mathcal{N}$ [23]. In our work, we derive assuming the left Jacobian (13); yet as presented in [23], it is also possible to compute the right Jacobian. For the case of SE(3), the Jacobian of the function $f$ will transform a vector of dimension $n$ to a vector in $\mathbb{R}^6$. Similarly, to functions mapping between Euclidean spaces, we can apply the chain rule given functions that map between manifolds. Given $Y = f(X)$ and $Z = g(Y)$, the Jacobian of $Z = g(f(X))$ is defined

$$J = \frac{DZ}{DX} = \frac{DZ}{DY} \frac{DY}{DX} = \frac{D(g(Y))}{DY} \frac{D(f(X))}{DX},$$ (14)

by the concatenation of the Jacobians of each function.
A.1.1 Gradient flow through our proposed SE(3)-DiF architecture (Sec. 3.2)

The proposed energy function in Sec. 3.2 takes as input an SE(3) element \( H \in \text{SE}(3) \) and outputs a scalar value \( E_{\theta} : \text{SE}(3) \rightarrow \mathbb{R} \). We model the energy function in two steps. First, we apply a rigid motion action over a set of points \( p \in \mathbb{R}^3 \)

\[
p' =Rp + t
\]

with \( R \in \text{SO}(3) \) and \( t \in \mathbb{R}^3 \) the rotation matrix and translation vector in \( H \) and \( p' \in \mathbb{R}^3 \times N \), the moved points. Then, we evaluate the cost of the moved points on a parameterize function \( e = c_\theta(p') \). From the architecture Fig. 3, the function is \( c_\theta(p') = D_\theta(F_\theta(H^p_0 p')) \). We compute the derivative of the energy function \( e = E_\theta(H) \) applying the chain rule

\[
\frac{De}{D\hat{H}} = \frac{De}{Dp'} \frac{Dp'}{D\hat{H}}
\]

where \( De/Dp' = \partial e/\partial p' \) is just the gradient of \( e \) w.r.t. \( p' \). On the other part, we can compute the Jacobian of the rigid motion action \( \frac{Dp'}{D\hat{H}} \) as presented in [23, 2].

A.1.2 A practical approach to computing the derivatives through SE(3)-DiF

In the following, we introduce a practical method to compute the derivative w.r.t. a Lie group element, that has previously been applied in the literature [6, 25]. This approach fails to consider the curvature of the manifold. Nevertheless, in practise, it allows the use of regular automatic differentiation tools. To compute the gradient, we first move \( H \in \text{SE}(3) \) to the Cartesian vector space \( h = \text{Logmap}(H) \). Then, we compute the energy function given \( h \)

\[
e = E_{\theta}(\text{Expmap}(h)).
\]

We compute the gradient of \( e \) w.r.t. \( h \) by regular backpropagation

\[
\frac{\partial e}{\partial h} = \frac{\partial e}{\partial p'} \frac{\partial p'}{\partial \text{Logmap}^{-1}} \frac{\partial \text{Logmap}^{-1}}{\partial h}.
\]

Similarly to (16), \( \partial e/\partial p' \) is a gradient of shape \( \mathbb{R}^3 \). Then, the Jacobian \( \partial p'/\partial \text{Logmap}^{-1} \) maps the gradient to \( \mathbb{R}^{4 \times 4} \). Taking a \( 4 \times 4 \) gradient might move the SE(3) element out of the manifold. To avoid it, we project the \( 4 \times 4 \) matrix to the Cartesian vector space \( \mathbb{R}^3 \) using the Jacobian \( \partial \text{Logmap}^{-1}/\partial h \). We have observed good performance when applying it in practise.

A.2 Distributions on Lie groups

To apply the score matching loss, we first sample a datapoint from a Gaussian distribution \( q_{\sigma_k}(\hat{x}|x) = \mathcal{N}(\hat{x}|x, \sigma_k I) \) with the mean \( x \sim \mathcal{N}(\hat{x}|x, \sigma_k I) \) sampled from the data distribution. A sample from \( q_{\sigma_k}(\hat{x}|x) \) can be easily obtain by perturbing a datapoint from the demonstrations with white noise \( \hat{x} = x + \epsilon \) with \( \epsilon \sim \mathcal{N}(0, \sigma_k I) \). Nevertheless, given SE(3) is not an Euclidean space, we cannot directly sample from a Gaussian distribution as the generated sample might fall out of the manifold. In our work, we adapt the Gaussian distribution to Lie Groups. Similarly to [24], we model the sampling distribution in SE(3) as

\[
q_{\sigma_k}(\hat{H}|H) \propto \exp \left( -\frac{1}{2} \| \text{Logmap}(H^{-1} \hat{H}) \|_{\Sigma^{-1}}^2 \right),
\]

where \( \Sigma = \sigma_k^2 I \) the covariance matrix. Following the intuition from [24], as long as \( \sigma_k \) is small enough, the tails of the distribution decay to zero along every geodesic path leading away from identity. We can sample from (19),

\[
\hat{H} = H \text{Expmap}(\epsilon), \quad \epsilon \sim \mathcal{N}(0, \sigma_k I),
\]

by first converting a white noise sample to a SE(3) element, and then, perturbing the mean of the distribution \( H \) with transformed white noise.
A.2.1 Score function in SE(3)

The score matching loss encourages the gradient of the parameterized model \( D \theta p \mathcal{H} \quad \text{to match the score of the perturbed distribution (19). We call } \phi = \text{Logmap}(H^{-1} H) \quad \text{and } M = H^{-1} H. \quad \text{We compute the score function by the chain rule}

\[
\frac{D \log q_{\sigma_k}(H | H)}{DH} = \frac{D(-\frac{1}{2} \| \phi \|^2_{\Sigma^{-1}})}{D \phi} \frac{D(\text{Logmap}(M))}{DM} \frac{D(H^{-1} H)}{DH}. \quad (21)
\]

The first part can be directly computed in the Euclidean space

\[
\frac{D(-\frac{1}{2} \| \phi \|^2_{\Sigma^{-1}})}{D \phi} = \frac{\partial}{\partial \phi}(-\frac{1}{2} \| \phi \|^2_{\Sigma^{-1}}) = -\frac{\phi}{\sigma_k^2}
\]

(22) that is the score function of a Gaussian distribution on Euclidean spaces. This is the score that is matched in [19]. The second term

\[
\frac{D(\text{Logmap}(M))}{DM} = J_l^{-1}(\phi)
\]

(23) is the inverse left-Jacobian on SE(3). See [2] Eq. (23-25). The third term

\[
\frac{D(H^{-1} H)}{DH} = \text{Adj}_{H^{-1}}
\]

(24) is the adjoint over \( H^{-1} \) (See [2] Eq. (17-21)).

B Algorithmic details

In this section, we provide the pseudocode for all 3 main algorithms (for training the diffusion models, for generating grasp poses, and for handling motion optimization with diffusion).

B.1 Algorithmic implementation of the training procedure

Algorithm 1 summarizes the training procedure for obtaining our SE(3)-DiF diffusion models. This section thus complements Sec. 3.2. Before starting to explain the training procedure, we want to point out that we are dealing with a combined objective (line 16). On the one hand, we refine the representation to learn the object’s sdf. Learning the sdf should instill geometric reasoning into the proposed architecture. In the algorithm, all operations that are related with this part are commented with “SDF”. On the other hand, our model should also be capable to match the score of the perturbed data distribution. Therefore, we use the denoising score matching loss as the second objective. All operations related to diffusion are marked with "DIF".

In every training iteration, we first sample a minibatch of \( b \) object ids. Next, we query the shape codes for all the selected objects. Please note that the shape codes are also learnable parameters, and actually updated during the training procedure. Afterwards follow the typical steps for learning the sdfs’ of the selected object, i.e., sampling j 3D points per object and their groundtruth sdf values, before querying the predictions by the network and constructing the loss function. From line 7 on follow the steps for score matching. We first start by sampling i grasp poses per object from the Acronym dataset [17]. The dataset originally contains good (successful) and bad (unsuccessful) grasping poses. However, as we are only interested in learning the distribution of successful grasping poses, we do not consider the bad ones in this sampling step. Next follow the steps of sampling noise and perturbing the previously selected grasping poses (lines 8-10). Following our explanations in Sec. 3.2, we represent the SE(3) grasping poses through a collection of \( N \) 3D points that are sampled around the gripper’s pose. We subsequently query our architecture to receive the features for each of these 3D points representing the grasping pose. Subsequently, we combine all of these points corresponding to a single grasping pose through flattening to obtain the predicted grasp quality (i.e., energy). We finally compute the DSM loss function, add the two objectives and perform gradient descent to update our network’s parameters as well as the object’s shape codes.
Algorithm 1: Training procedure for SE(3)-DiF

Given: \( \theta_0 \): initial parameters of the function \( E_{\theta} \);
S: Optimization steps;
Dataset \( D \) : \( \{ \{ H_{k,i} \}_{k=0}^{1}, \{ x_{k,j}, sdf_{k,j} \}_{j=0}^{b}, o_k \}_{k=0}^{K} \) : \( K \) objects, \( J \) 3D points \( x_{k,j} \in \mathbb{R}^3 \) per object with the sdf \( \text{ sdf}_{k,j} \) \( \in \mathbb{R} \) SDF value for each point, \( I \) \( H_{k,i} \in \text{SE}(3) \) good grasp poses per object, \( o_k \in \mathbb{R} \) object id.; \( H_{0}^{\nu_{0}} \) : object’s pose set to identity for training.

\[
\text{for } s \leftarrow 0 \text{ to } S - 1 \text{ do}
\]

1. \( o_{b} \in D; \) // Sample a minibatch of \( b \) objects ids
2. \( z_{b} = \text{shape codes}(o_{b}, \theta_{b}); \) // get all shape codes (see Fig. 3)
3. \( x_{b,j}, \text{ sdf}_{b,j} \in D; \) // SDF: Sample a minibatch of \( j \) 3D points and sdf per object
4. \( \text{ sdf}_{b,j}, - = F_{\theta}(x_{b,j}, z_{b}, k); \) // SDF: get predicted sdf (see Fig. 3)
5. \( \text{ sdf}_{b,j}, = \text{L}_{\text{sdf}}(\text{ sdf}_{b,j}, \text{ sdf}_{b,j}); \) // SDF: compute sdf error
6. \( H_{b,i} \sim D; \) // DIF: Sample a minibatch of \( i \) grasp poses per object
7. \( k, \sigma_{k} \leftarrow [0, \ldots, L]; \) // DIF: Sample a noise level
8. \( \epsilon_{b,i} \sim N(0, \sigma_{k}); \) // DIF: sample a white noise
9. \( \hat{H}_{b,i} = H_{b,i, \text{Expmap}}(\epsilon_{b,i}); \) // DIF: perturb grasp poses eq. (6)
10. \( x_{b,i,n}^{\nu} = H_{b,i, \text{Expmap}}(\epsilon_{b,i}); \) // DIF: Transform N 3d points (see Fig. 3)
11. \( \text{ sdf}_{b,i,n} = F_{\theta}(x_{b,i,n}, z_{b}, k); \) // DIF: get latent features (see Fig. 3)
12. \( \Phi_{b,i} = \text{Flatten}(\text{ sdf}_{b,i,n}, \Phi_{b,i}); \) // DIF: Flatten the features (see Fig. 3)
13. \( \epsilon_{b,i} = D_{\Phi}(\Phi_{b,i}); \) // DIF: Compute energy (see Fig. 3)
14. \( l_{\text{dim}} = \text{L}_{\text{dim}}(\epsilon_{b,i}, \hat{H}_{b,i}, H_{b,i}, \sigma_{k}); \) // DIF: Compute dsm loss with eq. (6)
15. \( l = l_{\text{dim}} + l_{\text{sd}}; \) // Sum losses
16. \( \theta_{s+1} = \theta_{s} - \alpha \nabla_{\theta} l; \) // Update parameter \( \theta \)

17. return \( \theta^{*} \);

B.2 Algorithmic implementation of 6D grasp generation using SE(3)-DiF

In Algorithm 2 we provide pseudocode for SE(3) grasp generation, closely following Sec. 3.1. We nevertheless want to point out that in some experiments in which also table collisions have to be considered, \( E_{\theta} \) might consist of multiple terms and therefore not only represent the energies output by our learned diffusion model.

Algorithm 2: SE(3) grasp generation pipeline

Given: \( \{ \sigma_{k} \}_{k=0}^{L} \) : Noise levels;
\( L \) : Diffusion steps;
\( \epsilon \) : step rate;
Initialize \( n_{s} \) initial samples \( H_{L}^{\nu_{0}} \sim p_{L}(H) \)

\[
\text{for } k \leftarrow 0 \text{ to } L - 1 \text{ do}
\]

1. \( e_{n_{s}} = E_{\theta}(H_{L}^{\nu_{0}}, k); \) // Compute the energy per \( H_{k}^{\nu_{0}} \)
2. \( \alpha_{k} = \epsilon \cdot \sigma_{k}; \) // Select step size \( \alpha_{k} \)
3. \( \epsilon \sim N(0, I); \) // Sample white noise vector of size \( \mathbb{R}^{6} \)
4. \( H_{k-1}^{\nu_{0}} = \text{Expmap} \left( - \frac{\alpha_{k}^{2}}{2} \frac{D_{\nu_{0}}}{D_{\nu_{0}}} + \alpha_{k}, \epsilon \right) H_{k-1}^{\nu_{0}}; \) // Make a 1d step
5. \( H_{0}^{\nu_{0}} \)

B.3 Algorithmic implementation of robot trajectory optimization using SE(3)-DiF

Algorithm 3 summarizes the procedure for trajectory optimization using inverse diffusion. The pseudocode follows Sec. 3.3. Again, the total cost per trajectory is usually a combination of multiple cost terms. Finally, we only return the minimum cost trajectory and execute it in simulation / on the real robot.

C Extended description of SE(3)-DiF’s architecture
Algorithm 3: Trajectory optimization pipeline

Given: \(\{\sigma_k\}_{k=1}^L\): Noise levels;
\(L\): Diffusion steps;
\(T\): trajectory length;
\(Q\): dimension of the configuration space;
\(\epsilon\): step rate;

Initialize \(n_s\) initial samples \(\tau^n_{k} \sim p_L(\tau)\) of size \(Q \times T\) each

1. for \(k \leftarrow L\) to 1 do
2. \[c_n = J(\tau^n_k, k)\] // Compute the total cost per \(\tau^n_k\)
3. \[\alpha_k = \epsilon / \sigma_k;\] // Select step size \(\alpha_k\)
4. \[\epsilon \sim N(0, I);\] // Sample white noise vector of size \(\mathbb{R}^{Q \times T}\)
5. \[\tau^n_{k-1} = \tau^n_k + \frac{1}{2}\alpha_k^2 \nabla \tau^n_k c_n + \alpha_k \epsilon;\] // Make a ld step
6. return \(\arg \min_{n_s} J(\tau_0^n, 0)\);

In the following we provide additional details on the architecture of our proposed SE(3) diffusion model for 6D grasp generation. This section adds additional details to Sec. 3.2. The internal architecture used to represent the feature encoder \(F_\theta\) in Fig. 3 and Fig. 12 is presented in Fig. 7. The architecture is composed of 8 fully-connected neural network layers, with hidden dimension of 512 and ReLU activation function. The architecture is based on DeepSDF’s architecture [27]. On the other hand, the decoder network \(D_\theta\), presented in Fig. 6, is a two-layer fully connected neural network with a hidden dimension of 512 and ReLU activation functions. For the pointcloud conditioned version (introduced in app. D.4), we used a Vector Neuron Pointnet [62] as the pointcloud encoder \(E_\theta\).

Figure 6: Internal architecture of the decoder \(D_\theta\). See the decoder in connection with other parts of the network in Fig. 3 and Fig. 12. The network first flatten the output of shape \(N \times (1 + 7)\) with \(N\) the number of points representing the grasp pose. In practise, we selected \(N = 30\).

Figure 7: Internal architecture of the feature encoder \(F_\theta\). See the feature encoder in connection with other parts of the network in Fig. 3 and Fig. 12. The used architecture is based on the one DeepSDF [27]. Our feature encoder extends the DeepSDF architecture with a \(k\) input variable, that represents the noise level of the diffusion model and the \(\psi\) variable that extracts additional features to learn the SE(3) grasp distribution.

D Extended experimental evaluation

D.1 Evaluation of SE(3)-DiffusionFields as 6D grasp pose generative models

In the following, we provide an extended presentation of the experiment in Sec. 4.1. We measure the success rate with the physics simulator Nvidia Isaac Sim. We present a visualization of the evaluation environment in Fig. 8. To evaluate the success rate of each model, we first generate 200 SE(3) grasp poses with each model and for each object. As we can observe in Fig. 8, the generated grasps are diverse and consider multiple grasping points. For our model, we get the initial SE(3) elements by sampling from a normal distribution on Lie groups

\[H_0 = \text{Expmap}(\epsilon), \quad \epsilon \sim N(0, \sigma I)\] (25)
with \( \sigma = \sigma_K \), the biggest noise level during the training. Then, we evaluate the grasps quality in Nvidia Isaac Gym. We reset the Franka’s end effector in the chosen grasp pose. We smoothly close the fingers until a tight grip is achieved and lift the gripper to a certain height. We consider the grasp to be successful if, after the lift, the mug remains close to the gripper. We also evaluate the divergence of the generated samples distribution w.r.t. data distribution. This divergence informs about how well the learned distribution matches the data distribution, covering all modes. We measure this divergence with the EMD [37]. We first sample \( N = 1000 \) grasp poses from the data distribution and from the learned model, respectively, and build a table with the relative distance between all the SE(3) grasp poses as

\[
d_{\text{SO}(3) + \mathbb{R}^3}(H_i, H_j) = \|t_i - t_j\| + \|\text{LogMap}(R_i^{-1} R_j)\|,
\]

with \( t_i \) and \( t_j \) the 3D position and \( R_i \) and \( R_j \) the rotation matrix of \( H_i \) and \( H_j \), respectively. Then, we solve a Linear Sum Assignment optimization problem [6]. This problem solves an optimal transport problem that will search for the least-distance one-to-one assignment between the samples in the data distribution and the sampled grasp poses from the learned model. The smaller the distance, the closer the generated samples are from the data distribution.

We compare the performance of SE(3)-DiF w.r.t. three models that are inspired by 6dof-GraspNet [6] and present the results in Fig. 4. We have trained a VAE to generate 6D grasp poses and a classifier to discriminate between good and bad grasp poses. The classifier network shares the same architecture of SE(3)-DiF, proposed in Fig. 3. For the VAE, we have trained a conditioned VAE that receives as input the shape code of the object to grasp and the 6D pose. We jointly train a DeepSDF [27] that shares the shape code with the conditioned VAE. We trained the classifier with a cross-entropy loss and added a gradient regularizer to encourage smoother gradients. Nevertheless, when the grasp poses are too far from the data distribution, the classifier lacks informative gradients that would allow us to move the grasp poses to the high-probability regions (See Fig. 4).

### D.2 Evaluation of SE(3)-DiffusionFields for robot grasp pose generation

This section complements the findings presented in Sec. 4.2. The results for the robot grasp pose generation have also been obtained in Nvidia Isaac Gym, using the procedure as shown in Fig. 9.

For obtaining the results, the optimizations not only consider the grasp pose in SE(3), but also the robot joint configuration. In particular, for the two end-end approaches, i.e., classifier & joint opt, we aim to minimize the following objective function

\[
J(q) = E_\theta(\phi_{\text{ee}}(q)) + c_{\text{table coll}}(q)
\]

with the learned grasp costs \( E_\theta \) and the table collision cost. The table collision avoidance cost is computed for all the collision spheres in the robot \( \mathbf{x}_c = (x_c, y_c, z_c) \in \mathbb{R}^3 \). Given the radius for a particular collision body is \( r_c \in \mathbb{R} \)

\[
c_{\text{table coll}}(q) = \sum_{c=0}^{K} \text{ReLU}(-(z_c - z_{\text{table}} - r_c)).
\]

For the separate optimization procedure, we first only optimize for the grasp poses \( H_{\text{grasp pose}} \) through

\[
J(H_{\text{grasp pose}}) = E_\theta(H_{\text{grasp pose}}),
\]
Figure 9: Visualization of evaluation procedure for robot grasp pose generation. Note that the pictures illustrate the evaluation of the 5 lowest cost particles using our proposed joint optimization with SE(3)-DiF. Importantly, each particle is evaluated in its own environment (environment is identified by colored arm & mug) and there are no collisions between different environments. Left to right: 1) All environments start with the same initial mug & robot pose. 2) Setting the arms to the optimized robot grasp pose. 3 & 4) Attempting to lift the mugs. In this case, all the particles result in successes.

d thereby not taking into account the current pose of the object, nor any other environmental constraint and thus have to subsequently optimize the following cost function in joint space (for fixed $H_{\text{grasp pose}}$)

$$J(q) = c_{\text{des grasp dist}}(\phi_{ee}(q), H_{\text{grasp pose}}) + c_{\text{table coll.}}(q)$$

with current grasping pose $H(q)$ and the cost on the distance to the previously optimized grasp pose

$$c_{\text{des grasp dist}}(H(q), H_{\text{grasp pose}}) = 10\|q - q_{\text{grasp pose}}\| + \|\text{LogMap}(R_q^{-1}R_{\text{grasp pose}})\|.$$  

Note the additional factor of 10 due to the different scales of position error in $[m]$ and orientation error in $[\text{rad}]$.

As we have shown in the main paper (cf. Sec. 4.2), and as it is also underlined by the accompanied videos (accessible in the linked website in the abstract), using the classifier, and the separate optimization performs substantially worse performance compared to our proposed joint optimization using SE(3)-DiF.

For the separate optimization procedure (sample + opt), we actually even ran two variants. The results of optimizing ten joint configuration samples per previously sampled grasp pose ($n_{sm} = 10$) have been shown in the main paper, thus the second optimization phase even considers 1000 samples in total (100 grasping poses × 10 samples per grasp pose). When comparing these results to only optimizing one joint configuration per grasp in the second stage ($n_{sm} = 1$), we observe that optimizing for finding the single desired grasp pose while also avoiding table collisions is difficult. Allowing 10 joint configuration samples per grasp pose and only evaluating the best one ($n_{sm} = 10$) performs substantially better, but still worse compared to our proposed joint optimization with SE(3)-DiF. Particularly, the experiments showcase a performance drop w.r.t. the flipped mug scenario. This underlines the major shortcoming of not being adaptive w.r.t. the current environment. The split optimization for grasp pose and joint configuration results in many proposed grasp poses which are simply infeasible. Contrarily, for our proposed joint optimization the ratio of overall successful particles $s_{\Omega}$ drops only slightly, and even remains on the same high level of 0.88. We, thus, conclude that end-end gradient-based optimization with our SE(3)-DiF model results in highly performant, reliable, and adaptive robot grasp pose generation, despite the multi-objective scenario.

**Exact weighting of cost terms**

In Table 3, we additionally present the exact weighting of the cost terms that have been used for generating the results presented in Sec. 4.2 & App. D.2.

Table 2: Comparing different approaches for robot grasp pose generation with $n_s = 100$ initial samples.

| Method                  | Objects upright $s_{\Omega}$ | Objects flipped $s_1$ |
|-------------------------|-------------------------------|------------------------|
| joint opt (classifier)  | 0.03                          | 0.03 (0.68)           |
| sample (SE(3)-DiF) + opt ($n_{sm} = 1$) | 0.11                          | 0.03 (0.57)           |
| sample (SE(3)-DiF) + opt ($n_{sm} = 10$) | 0.46                          | 0.12 (0.76)           |
| **Ours**                | **0.62**                      | **0.88**              |
Table 3: This table summarizes the weighting of the individual cost terms that have been used for generating robot grasp poses, as presented in Sec. 4.2 & App. D.2. The table’s first two rows describe the weighting of the cost terms when running one single joint optimization procedure in which grasp generation and avoiding table collisions are considered jointly. While for the method in the first row, we use the trained classifier as described in Sec. 4.2, all the other approaches use our proposed SE(3)-DiF diffusion model as the cost function for evaluating grasp poses. Moreover, table’s last two rows detail the weighting of the cost terms for the split, two-stage optimization procedure. Note that the separate optimization thus requires running two optimizations.

![Figure 10: Scenarios for Picking with occlusions. The boxes and the table are obstacles and the robot must find a trajectory to grasp the mug. We consider the mug might be positioned both upright and upside-down.](image)

### D.3 Evaluation of SE(3)-DiffusionFields for joint grasp and motion optimization

In the following, we provide an extended presentation of the experiments in Sec. 4.2. We evaluate the performance of SE(3)-DiF as cost function in a trajectory optimization problem. We consider three robot tasks in which both the selection of the grasping pose, and the trajectory planning are required. We explore if we can use SE(3)-DiF as a cost in a single trajectory optimization problem and jointly optimize both for the trajectory and the grasp pose at the last waypoint. The objective function

\[
J(\tau, k) = E_\theta(\phi_{ee}(q_{t:T}), k) + \sum_k c_k(\tau)
\]  

(32)

is composed of both the learned SE(3)-DiF, \(E_\theta\) and a set of heuristics cost functions that represent different subtasks (trajectory smoothness, collision avoidance, ...). All trajectories are planned in the configuration space. Then, we frame the optimization problem as an inverse diffusion process and diffuse a set of initial trajectory samples as presented in Sec. 3.3. We sample the initial trajectories as straight trajectories in the configuration space towards a randomly sampled configuration. After diffusing a set of trajectories, we pick the one with the lowest accumulated cost, \(J(\tau, 1)\). We evaluate this approach in three tasks that require the planning of both the trajectory and the grasping pose: picking an object with occlusions, picking and reorienting an object and pick and placing on shelves.

#### D.3.1 Picking with occlusions

In the following, we provide an extended presentation of the experiment on picking an object with occlusions. The experimental evaluation is performed in three different scenarios, with the mug initialized both in normal pose or upside down. We illustrate the scenarios in Fig. 10. We evaluate the success for 100 trajectories with different mugs positions for the three environments. The success is measured by following the generated trajectory. Once the robot is in the last position of the generated trajectory, we close the fingers. We consider a success case if the mug is in contact with both fingers once the fingers close.
The objective function for this problem is defined by the following cost functions: (a) Grasp Pose SE(3)-DiF over the final configuration $q_f$, (b) a trajectory smoothness cost, (c) a table avoidance cost, (d) box avoidance costs, (e) initial configuration fixing cost and, (f) a pregrasp cost. Given some of the costs are defined in the task space, we use a differentiable robot kinematic model, based on Facebook’s kinematics model [9]. We define the collision body of our robot by a set of spheres similar to [10]. We set the trajectory smoothness cost

$$c_{\text{smooth}}(\tau) = \sum_{t=1}^{T-1} \|q_{t+1} - q_t\|^2$$

(33)

as the minimization of the relative distance between the neighbour points in the trajectory. This cost can be thought as a spring making all the points in the trajectory be attracted between each other. The table collision avoidance cost is computed for all the collision spheres in the robot $x_{ct} = (x_{ct}, y_{ct}, z_{ct}) \in \mathbb{R}^3$. Given the radius for a particular collision body is $r_c$

$$c_{\text{table\,coll.}}(\tau) = \sum_{t=1}^{T} \sum_{c=0}^{K} \text{ReLU}(- (z_{ct} - z_{\text{table}} - r_c)) \tag{34}$$

with $z_{\text{table}}$ the height of the table and a Rectified Linear Unit (ReLU) to bound the cost. Given we have access to the SDF of the collision obstacles in the environment, we can set the box collision cost as

$$c_{\text{box\,coll.}}(\tau) = \sum_{t=1}^{T} \sum_{c=0}^{K} \text{ReLU}(- (\text{SDF}(x_{ct}) - r_c)) \tag{35}$$

In the trajectory optimization problems, we might want to fix the initial configuration to the current robot configuration. While the easiest approach is not updating $q_0$ during optimization, we can alternatively set the initial configuration fixing cost

$$c_{\text{fix}}(\tau) = \|q_1 - q_{\text{init}}\|$$

(36)

with $q_{\text{init}}$ the initial configuration of the robot. Finally, we set also a pregrasping cost. It is common to approximate to the grasp in the cartesian space from a grasp a few centimeters over the grasp pose. We set a cost that encourages the optimized trajectory to approximate in this way

$$c_{\text{pregrasp}}(\tau) = \sum_{t=T-n}^{T-1} d_{\text{SO(3)+R^3}}(H_{ee,t}, H_{\text{pre},t})$$

(37)

with $H_{ee,t}$ the end effector pose in the instant $t$ and $H_{\text{pre}} = H_{ee,T} H_{z,t}$ a pose that is to a certain distance over the $z$ axis from the final pose.

As baseline, we also evaluate the performance of solving the task in a hierarchical approach. In this case, we first sample a SE(3) grasp pose given our learned SE(3)-DiF and then, we solve the trajectory optimization problem, given the target grasp pose is fix with the cost $d_{\text{SO(3)+R^3}}$. The complete evaluation can be found in Fig. 11.

We evaluate the success rate of the model assuming a different set of initial particles. We observe that the performance in all the cases increases when considering more initial particles. Gradient based motion optimization is an inherently locally optimization method and therefore, its performance is
highly influenced by the initialization. To enhance the performance, multiple initial particles, initialized in different states might explore better the optimization field and find more optimal solutions. We observe that the joint optimization approach outperforms the hierarchical approach in all the cases. This is expected solution. A hierarchical approach decouples the grasp selection from the trajectory optimization. Then, if the selected grasp is unfeasible for the robot, we will not be able to find a good trajectory. Instead a joint optimization problem iteratively updates the trajectory improving both the grasp cost and the rest of the costs. Therefore, we find that jointly optimizing is more sample efficient than a hierarchical approach.

**Exact weighting of cost terms**

In Table 4 we present the weighting of the individual cost terms that we have used to obtain the trajectories for these scenarios of having to pick the mug under occlusions.

| Description                     | Cost                                   | Weight |
|---------------------------------|----------------------------------------|--------|
| Grasp pose evaluation           | \( \mathcal{E}(\theta, q_\theta, k) \) | 5      |
| Trajectory smoothness           | \( \mathcal{\text{smooth}}(\tau) \)    | 10     |
| Table collision avoidance       | \( \mathcal{\text{table coll}}(\tau) \) | 20     |
| Box collision cost (other obstacles) | \( \mathcal{\text{box coll}}(\tau) \) | 20     |
| Initial configuration fixing cost | \( \mathcal{\text{fix}}(\tau) \)         | 10     |
| Pregrasping cost                | \( \mathcal{\text{pregrasp}}(\tau) \)   | 5      |

Table 4: This table summarizes the weighting of the individual cost terms that have been used for generating robot trajectories for the task of picking a mug under occlusions, as presented in Sec. 4.2 & App. D.3.1.

**D.3.2 Pick and reorient**

In the following we provide an extended presentation of the experiment of picking and reorienting an object. This experiment aims to explore the performance of SE(3)-DiF in a complex manipulation task as the one of picking an object and reorient it. We highlight that the whole optimization problem on how to grasp the object, and how to move it to a target pose is solved in a single optimization loop. The problem is interesting as the optimized trajectory should not only consider that there is a collision free path to an affordable grasp pose, but also, that the chosen grasp pose allows us to put the object in a desired target pose. We evaluate the performance of our model 100 times in which the objects are initialized in an arbitrary random pose and have to be placed in an arbitrary placing pose. We consider a trial to be successful, if after executing the whole trajectory, the distance between the grasped object and target pose is smaller to a threshold.

The objective function for this problem maintains multiple costs from the pick on occluded problem (trajectory smoothness, pregrasp, initial target fix, table collision). Additionally, we consider the grasp SE(3)-DiF at the instant \( t = T/2 \) (we aim to grasp an object in the middle of the trajectory). Finally, we want to impose that the relative position of the object with respect to the gripper in the grasping moment should be the same as the relative position in the placing. We impose this by first computing the pose in the object’s frame \( \mathcal{H}_{ee,t} = (\mathcal{H}_{w,t}^{-1}) \mathcal{H}_{ee,t} \), with \( \mathcal{H}^{w}_{ee,t} \) being the end effector pose in the world frame at the instant \( t \) and \( \mathcal{H}^{w}_{oo,t} \) the pose of the object in the world frame at the instant \( t \). We define the **grasp-place pose similarity cost** as \( \mathcal{c}_{\text{grasp-place similarity}}(\tau) = d_{\mathcal{SO}(3) \times \mathbb{R}^3}(\mathcal{H}^{w}_{ee,T/2}, \mathcal{H}^{w}_{ee,T}) \), that encourages the end effector pose w.r.t. the object frame to be the same in both the grasping moment and the placing moment.

**Exact weighting of cost terms**

In Table 5 we present the weighting of the individual cost terms that we have used to obtain the trajectories for these scenarios of having to pickup a mug and reorienting it to fullfil a desired final pose.

**D.3.3 Pick and place on shelves**

In the following, we provide an extended presentation of the experiment of picking and placing on shelves. Similarly to the pick and reorient task, this experiment was chosen to evaluate the performance of SE(3)-DiF solving complex manipulation tasks jointly. This task is of high interest as both the set of affordable grasping poses and placing poses is very small due to the possible collisions with the shelves and therefore, jointly optimizing the trajectory and the grasp pose might
Table 5: This table summarizes the weighting of the individual cost terms that have been used for generating robot trajectories for the task of picking a mug in the first half of the trajectory and reorienting it to a desired final pose in the second half of the trajectory, as presented in Sec. 4.2 & App. D.3.2.

Table 6: This table summarizes the weighting of the individual cost terms that have been used for generating robot trajectories for the task of picking and placing a mug inside a shelf as presented in Sec. 4.2 & App. D.3.3.

D.4 Pointcloud based SE(3)-DiffusionFields

The presented work is focused on evaluating the performance of diffusion models as both 6D grasp generative models and cost functions in trajectory optimization. Thus, to avoid perception related uncertainty, in this work, we assume the object shape and pose are known. We assume that we can rely on state-of-the-art object pose detection and segmentation to estimate the object class and...
Figure 13: Evaluation of the Success for picking with occlusions. PoiNt-SE(3)-DiF refers to the model with a pointcloud encoder, SE(3)-DiF (Rot) to the model in which the pose is infer from the pointcloud, SE(3)-DiF the model in which both the pose and shape are known, SE(3)-DiF (Z+Rot) the model in which both the object pose and shape codes are inferred from the pointcloud, and 6DoF-Graspnet [6].

We apply an autodecoder approach [27] and learn a set of latent codes $z$ that represent the different shapes. Then, in practice, given we know the exact object, we can retrieve the shape code $z$ given we know the index of the object.

For completeness, in this experimental section, we evaluate the performance of SE(3)-DiF with a Pointcloud encoder instead of an autodecoder. We modify the architecture in Fig. 3 and add a pointcloud encoder $E_{\theta}$. We refer to this model as PoiNt-SE(3)-DiF. We present the modified architecture in Fig. 12. We model the pointcloud encoder $E_{\theta}$ with a VN-PointNet [62]. The network outputs SO(3)-equivariant features that allow us to easily encode the orientation of the different objects. A similar network has been previously applied in [13] to learn the features of a graspable object.

We aim to evaluate the performance difference between the autodecoder-based SE(3)-DiF and the pointcloud encoder-based SE(3)-DiF models. We consider three scenarios for the autodecoder-based model: (i) Both object shape and pose are known, (ii) Only the shape is known and (iii) We don’t know either the shape nor the pose of the object. The case (i), where both pose and shape of the object are known, is presented in sec. 4.1. For the cases when either the object pose or both pose and shape code are unknown, we rely on pointclouds for inferring them. We follow a similar inference approach to the one proposed in [27] and extended it to infer also the pose of the object $H_{o}^{w}$. Given a pointcloud $P : \{x_n\}_{n=0}^{N}$ and the learned SDF function $F_{\theta}^{sdf}$, we infer the $H_{o}^{w}$ by

$$H_{o}^{w} = \arg\min_{H_{o}} \frac{1}{N} \sum_{n=0}^{N} F_{\theta}^{sdf}(H_{o}^{w} x_{n}, z)$$

(38)

given $z$ the shape code of a known object. Intuitively, (38) searches for the object pose $H_{o}^{w}$ that makes the pointcloud pose to match the one of the learned SDF function. We can think of this optimization problem as an Iterative Closest Point (ICP) algorithm [14], but instead of matching two sets of points, we match a set of points with the SDF function. For the case when neither pose nor shape of the object is known, we infer both $z$ and $H_{o}^{w}$

$$H_{o}^{w}, z^{*} = \arg\min_{H_{o}^{w}, z} \frac{1}{N} \sum_{n=0}^{N} F_{\theta}^{sdf}(H_{o}^{w} x_{n}, z) + \|z\|^{2},$$

(39)

and we extend the optimization for both the shape code $z$ and the object’s pose $H_{o}^{w}$. We additionally add a L2 regularizer over $z$ as proposed by [27].

We evaluate the performance of the autodecoder-based approaches and the pointcloud encoder-based model w.r.t. their success rate in generating successful grasps and the EMD. We additionally add 6DoF-Graspnet [6] as baseline to compare all the methods. We follow the same evaluation procedure from Sec. 4.1. We present the results of the evaluation in Fig. 13. In Fig. 13, we name SE(3)-DiF the case where both object shape and pose are known, SE(3)-DiF (Rot) the case where the object’s shape is known, and the pose is inferred by pointclouds with (38), SE(3)-DiF (Z+Rot) the case in which both object pose and shape are inferred with (39) and PoiNt-SE(3)-DiF the Pointcloud conditioned model. We observe a high performance in terms of both success rate and EMD for SE(3)-DiF, SE(3)-DiF (Rot) and for the PoiNt-SE(3)-DiF. We also observe that the best success rate and EMD was achieved by SE(3)-DiF, followed by SE(3)-DiF (Rot) and PoiNt-SE(3)-DiF. We hypothesize that this might be related to the unknown variables on each case. PoiNt-SE(3)-DiF needs to infer both the shape and the pose, while SE(3)-DiF assumes this to be known. We observe that SE(3)-DiF (Z+Rot) was not able to achieve a high success rate. We were not able to properly infer both
Figure 14: Performance comparison between computing the derivative w.r.t. a Lie group element [16] and computing the derivative by approximation [25] for training and evaluating SE(3)-DiF models. We performed the comparison following the experiment in Sec. 4.1. **Right:** success rate for grasping and lifting a mug. **Left:** Wasserstein distance (EMD) to the training distribution (lower is better).

The shape code and the pose jointly by (39). Therefore, if both the shape and the pose are unknown, we propose using PoInT-SE(3)-DiF, while if the shape and the pose are known, we rather propose using the autodecoder approach. We observe, that all diffusion-based methods, except the SE(3)-DiF (Z+Rot) outperformed 6DoF-GraspNet in terms of both success rate and Earth Mover Distance. While the success rate of 6DoF-GraspNet is close to the one of the diffusion models, the EMD decays alot. This evaluation infers that the samples obtained by 6DoF-GraspNet are less diverse and the generation collapses to some modes in the dataset without covering it all. Instead, diffusion based methods

D.5 Comparison between approximated derivatives and derivatives w.r.t. Lie group elements

In the following experiment, we evaluate the performance difference between different approaches to compute the derivative of (6). As introduced in App. A, the derivative w.r.t. Lie group elements requires additional insights in its computation. Most of the current state-of-the-art auto-differentiation tools (Pytorch’s autograd) [25] do not take into consideration the geometry of the manifold and instead only approximate the derivative. In this experiment, we compare the performance differences between training SE(3)-DiF with the approximated derivative and with the properly computed one. To integrate the derivatives w.r.t. Lie group elements with Pytorch’s autograd, we use the library Theseus [16].

We compare the methods by performing a similar experiment as presented in Sec. 4.1. We train two diffusion models to generate 6D grasp poses. Our dataset is composed of the successful grasping poses for 50 different mugs from the Acronym dataset [17]. We trained both models for 1400 epochs. The models are compared using Nvidia’s Isaac Gym simulator [36]. For each object in our dataset, we generate 40 grasp poses from each diffusion model. Then, we evaluate if the generated grasp pose is valid to pick the mug and lift it. We also evaluate the performance in terms of EMD. This distance measures the Wasserstein distance between the training dataset and the samples generated by our diffusion models. EMD indicates how well the generated samples cover all the modes of the training dataset (cf. Sec. 4.1).

We present the results in Fig. 14. As we can observe, both models show similar performance in terms of success rate. In terms of EMD (lower is better), we observe that the properly computed derivative results in lower variance, yet, the approximated derivative yields lower mean. The experiment thus indicates that in practise, for training and evaluating SE(3)-DiF models for grasp generation, both methods performed similarly. Note that for the experiment in Sec. 4.1 SE(3)-DiF and the other models have been trained for 10 times more epochs and then, the performance was also better.

D.6 Real robot experiments

In this part, we present the results of evaluating our proposed joint optimization using SE(3)-DiF in a range of real-world experimental setups. In Fig. 15, we display two exemplary setups. Additional videos can be found on our webpage. As can be seen in the figures, we use Optirack to retrieve the current mug pose. For all the experiments, we optimize the entire trajectory, thereby following
App. B.2. Overall, the experiments aim at assessing the method’s capabilities in realistic conditions that include, i) non perfect state information, as the mugs pose is retrieved from Optitrack and there might be small errors due to the calibration between the robot and Optitrack, ii) slight variations in the mug’s shape, as we use a mug that is slightly different from the model that we assume for grasp pose generation (therefore we assume the latent to be given and do not finetune it), and iii) trajectory execution in the real world, thereby we also investigate whether the proposed grasps from the Acronym dataset (i.e., the grasping data we trained on) do transfer to the real world or not.

In the following, we will briefly describe the individual experimental scenarios, before finishing this chapter with a summary of all the experiments. For videos, please see https://sites.google.com/view/se3dif.

D.6.1 Joint grasp and motion optimization for picking mugs without obstacles

Typical setups for this line of experiments are illustrated in Fig. 15a and Fig. 16. For generating the trajectories, we use our proposed joint optimization based on the learned SE(3)-DiF net (cf. App. B.3), and additionally take into account potential collisions with the table. In fact, we make use of the same cost function as presented in App. D.3.1 and only omit the cost on the other obstacles, except for the table. We use 800 initial particles (i.e., 800 entire trajectories) during the optimization process. While Fig. 15a displays a more regular scene as the mug is placed in its normal, upright pose, we also evaluate the flexibility of our method by placing the mug in more complicated poses. Nevertheless, due to the joint optimization, the approach adapts seamlessly, as shown in Fig. 16.

Quantitative results

For this experiment of having to pick a mug without any other conclusions, we also collected quantitative results. We consider two separate scenarios. In one, the mug is placed in its nominal upright position on the table. In the second one, we place the mug upside down. Thus, this experimental setup is intended to provide a comparison to the simulated ones in Sec. 4.1. Nevertheless, compared to Sec. 4.1, herein, we considered to optimize the robot’s entire trajectory and did not solely focus on the final grasping pose. The reason for this is that in reality we cannot simply set the robot to an arbitrary pose. In fact, the trajectory to the final desired grasping pose is a crucial component for a grasp to succeed. Moreover, we increased the number of initial particles to 800. Due to the significant effort for realizing real world experiments, opposed to the evaluation in Sec. 4.1, in both scenarios (mug in nominal / upside down pose) we only consider one type of mug. We nevertheless vary over 5 different initial mug positions and report the success rates for evaluating the best particle ($s_1$), as well as the 5 best particles ($s_5$), across these 5 different initial positions.

The results of this experiment are presented in Table 7. These real world results confirm the applicability of our proposed method. In fact, when only quantitative results

Table 7: Evaluating our proposed joint optimization on the trajectory level for picking up mugs in a real world setup. We make use of $n_s = 800$ initial samples, i.e., initial trajectories.

| Objects upright | Objects flipped |
|-----------------|-----------------|
| Method          | $s_1$ | $s_5$ | $s_1$ | $s_5$ |
| Ours            | 0.96  | 1.0   | 0.92  | 1.0   |

The results of this experiment are presented in Table 7. These real world results confirm the applicability of our proposed method. In fact, when only quantitative results

Figure 15: Illustrating two evaluation scenarios in the real world. We use Optitrack to retrieve the pose of the mugs. Fig. 15a shows a scenario without any other objects, whereas Fig. 15b corresponds to a pick and place under occlusion scenario. For all real robot evaluations we optimize the robot’s entire trajectory.
considering the evaluation of the best particle, we achieve a perfect success rate of 100%, i.e., all the 5 grasping trajectories are successful for the 5 different initial mug positions in both scenarios. When considering the evaluation of the 5 best particles (i.e., trajectories) we achieve 24/25 grasp successes for the mug placed in its nominal position and 23/25 for the scenario when the mug is placed upside down. Compared to the simulation-based experiments from Sec. Sec. 4.1 we remark that we attribute the increased performance to the significant increase in the number of particles, as well as to the reduced sample-size. Nevertheless, these results confirm that our proposed diffusion model and the proposed joint optimization scheme achieve high performance in real settings, despite potential noise from the object pose estimation pipeline, using slightly different mugs compared to the ones included in the dataset, as well as the fact that the Acronym grasps have been labelled in simulation.

D.6.2 Joint grasp and motion optimization for picking mugs with occlusions

We now consider a more complicated pickup scenario in which we add obstacles to the scene as shown in Fig. 15b. We thus have to augment the objective functions to also penalize potential collisions with the obstacles (cf. App. D.3.1). As in the previous line of experiments, we shoot 800 initial particles and only evaluate the best one. Fig. 15b depicts an exemplary successful trajectory in which the end effector moves in parallel to the box that is occluding the mug in order to avoid collisions, while still approaching a valid grasp pose that allows for lifting the mug.
Figure 19: Illustration of another trajectory for the pick and reorient scenario. While the robot is able to reorient the mug in its desired pose, along the way, we lose one of the Optitrack markers (frame c) due to a collision with the table. In the future, we therefore have to add more terms to our cost functions as this potential collision between mug and table, and even Optitrack marker and table are not reflected in the objective function’s current form. Thus, this failure is not directly related with our method, but rather with the choice of objective function.

D.6.3 Joint grasp and motion optimization for pick and reorient

Lastly, we consider the pick and reorient scenarios, as illustrated in Fig. 18 & Fig. 19. Therefore, we emphasize our method’s flexibility, as we can seamlessly add additional terms to the objective function that reflect future goals, even after having grasped the object. The overall objective function is again chosen as described in App. D.3.2. While Fig. 18 shows a successful trajectory, Fig. 19 reveals that our current choice of objective function is missing some terms. In particular, in this case, we lose one of the mug’s Optitrack marker due to a collision between this marker and the table. Despite loosing this one marker, we nevertheless still reach the complicated desired end pose.

D.6.4 Summary and limitations

Throughout all the real-world experiments, we find that our proposed joint optimization performs robustly and maintains the adaptivity that we already reported for the simulation experiments. The observed behavior also underline the expressivity of our objective functions, as their value decides on sorting the particles. Only in a few cases in the more complicated scenarios, we observe failures. However, these can mainly be attributed to unmodelled effects. For instance in the pick and reorient scenarios, as we do not consider the SDF of the mug after pickup, we sometimes obtain trajectories in which the mug collides with the table. In the future, we plan to incorporate these effects into the objective functions to further boost our method’s performance.

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