Flow Stochastic Segmentation Networks

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Abstract

We introduce the Flow Stochastic Segmentation Network (Flow-SSN), a generative segmentation model family featuring discrete-time autoregressive and modern continuous-time flow variants. We prove fundamental limitations of the low-rank parameterisation of previous methods and show that Flow-SSNs can estimate arbitrarily high-rank pixel-wise covariances without assuming the rank or storing the distributional parameters. Flow-SSNs are also more efficient to sample from than standard diffusion-based segmentation models, thanks to most of the model capacity being allocated to learning the base distribution of the flow, constituting an expressive prior. We apply Flow-SSNs to challenging medical imaging benchmarks and achieve state-of-the-art results. Code available: https://github.com/biomedia-mira/flow-ssn.

1. Introduction

Semantic image segmentation consists of producing pixel-wise predictions that reflect objects and their boundaries. Traditional methods typically approach this as a deterministic pixel-wise classification task, while overlooking the inherent *uncertainty* of the spatial structures involved [11, 36, 98]. Uncertainty generally relates to unknown or imperfect information, often arising from a lack of knowledge, partial observations, and/or inherently stochastic events. Uncertainty is commonly decomposed into two distinct parts [18, 36]: (i) *Epistemic* uncertainty, which relates to a lack of knowledge, and it can be reduced in principle by observing more data; (ii) *Aleatoric* uncertainty, which relates to inherent unknowns that differ each time we run the same experiment (e.g. flipping a coin), and it cannot be reduced by observing more data. Although conceptually attractive, the utility and validity of this decomposition is actively contested [41, 79].

Inherent ambiguities are particularly prevalent in medical imaging, where medical opinions can vary significantly across different experts [5, 9, 35, 43]. In this context, uncertainty can arise from several factors, including indistinct boundaries, occlusion, poor image acquisition quality, and the intrinsic variability of the underlying pathology. Therefore, to effectively model these ambiguities and reflect the real-world variability of expert opinions, segmentation models ought to capture a rich *distribution* of plausible segmentation outcomes [14, 43]. Furthermore, providing uncertainty estimates is useful for revealing whether a model has sufficient knowledge to provide a reliable assessment, which is important in safety-critical real-world settings [7, 47, 63].

There is a growing interest in using probabilistic methods for estimating uncertainty in image segmentation. Most existing methods handle uncertainty by factorising the output posterior into per-pixel marginal distributions, thereby ignoring any correlations between pixels. Therefore, pixel-wise independent uncertainty estimates are incapable of fully capturing spatially structured uncertainty [46, 58]. To address this, Monteiro et al. [55] proposed Stochastic Segmentation Networks (SSNs), which can explicitly model spatially correlated aleatoric uncertainty without requiring variational approximations or latent variable assumptions. Their method involves placing a low-rank multivariate Gaussian distribution over the logit space (i.e. before the softmax), then using Monte Carlo integration to marginalise out the logits and compute pixel-wise joint likelihoods [36, 37]. Although promising, the trouble with SSNs is three-fold: (i) The assumed rank of the low-rank approximation is typically kept small due to computational constraints (e.g., $\simeq$10), and it is almost surely underspecified relative to the true rank of high-dimensional, pixel-wise covariances; (ii) They often require an expensive mean pre-training stage to ensure proper convergence, as jointly optimising poor initial estimates of the mean and covariance can lead to getting trapped in sub-optimal minima; (iii) They suffer from training instabilities, partly due to a lack of guarantee that the low-rank covariance matrix remains positive definite throughout training.

Contributions. We propose Flow Stochastic Segmentation Networks (Flow-SSNs), a generative segmentation model class featuring discrete-time autoregressive and modern continuous-time flow parameterisations. Flow-SSNs can estimate arbitrarily high-rank pixel-wise covariances without assuming the rank a priori, storing distributional parameters, or assuming a lower-dimensional latent space as in VAEs.

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Flow-SSNs are more efficient to sample from than typical diffusion-based segmentation models, as most of the model capacity is dedicated to learning a flow's *prior*, while the flow itself is lightweight. In summary, our contributions are:

- §4 We prove fundamental limitations of the low-rank parameterisation of SSNs by showing that the effective rank grows sublinearly with the assumed rank;
- §5 We introduce Flow-SSNs, a generative segmentation model capable of modelling complex covariance structures efficiently by learning a flow's *prior* and using a lightweight flow to model pixel-wise dependencies;
- §6 Applying Flow-SSN to a toy problem and two real-world medical image segmentation benchmarks, we show state-of-the-art results with fewer parameters.

2. Related Work

Existing work on stochastic segmentation can be broadly categorised as: (i) Bayesian methods which approximate a posterior over neural network parameters [36]; (ii) latent variable generative models [6, 43, 89]; and (iii) distributional/evidential methods, which estimate a complex joint distribution directly in pixel space [53, 55, 77, 84]. Mackay [52], Neal [57] and Hinton and Van Camp [30] laid the foundations for modern-day Bayesian Neural Networks (BNNs), which approximate neural network parameter posteriors and enable uncertainty estimation. More recently, Kendall and Gal [36], Kwon et al. [45], and others [15, 16, 37, 90], used these techniques for classification/segmentation, but handled uncertainty by factorising the output posterior into per-pixel marginal distributions, thereby ignoring pixel correlations.

Stochastic segmentation methods based on the Variational Autoencoder (VAE) [39, 70] framework implicitly assume that the data resides in a lower-dimensional latent manifold and hope that the pixel-wise independent decoder will learn to translate uncorrelated latent variables into meaningful spatial variation in pixel space [6, 43, 93]. Selvan et al. [76], Valiuddin et al. [86] also use a VAE for segmentation but apply a normalising flow [81] to the latent variables to make them more expressive. Since providing latent variable identifiability guarantees is challenging for most problems [34], one often resorts to unfalsifiable assumptions about both the functional form and dimensionality of the latent space. Although VAEs can work well for certain segmentation tasks [43, 54], they sometimes underperform in high-dimensional settings, and are subject to the *prior hole* problem [27, 50, 69, 71].

Diffusion models [31, 80] are a promising viable alternative which has been recently explored for producing stochastic segmentations [3, 66, 89, 92]. However, their high inference costs can restrict their usability for medical experts to edit segmentation annotations in real-time. Recent work on Continuous Normalising Flows (CNFs) [12] provides efficient (simulation-free) ways to learn straighter paths between distributions compared to diffusion paths [2, 48, 49, 82]. CNFs that induce straighter paths are computationally more efficient to solve, making them an attractive option for real-time editing of medical imaging annotations. There is limited prior work on exploring CNFs for segmentation; [8] combine Flow Matching (FM) [48] with the signed distance function (SDF) for image segmentation, but their investigation is restricted to binary data. Our approach differs substantially in its formulation as it is defined within an SSN-like [55] paradigm, and naturally extends to categorical data. Specifically, our model generates multiple segmentations by sampling from an expressive, learned base distribution (i.e. prior) conditional on the image, rather than random noise.

Limited prior work exists on using autoregressive models for stochastic segmentation tasks. Zhang et al. [95] proposed an autoregressive approach using a PixelCNN [74, 87], which can learn full rank pixel-wise covariances. However, it requires each pixel to be generated sequentially, which is slow. To mitigate this, they use a downsampled resolution, discarding input information. SSNs [55] provide a simpler alternative for learning the joint distribution over pixel-wise label maps that does not require making latent variable assumptions or variational approximations. Multiple works build on SSNs to enable fine-grained sample control [59], learning mixtures of stochastic experts [24] and conditioning on label style [93]. However, SSNs are subject to training instabilities and make strong assumptions about the rank of the true pixel-wise covariance being quite small, which is under-determined for most problems. Flow-SSNs make no such assumptions and can estimate arbitrarily high-rank covariances. Concurrently, [28, 83, 94] revisit classical flow models [21, 38, 61] for generation, but not for segmentation.

3. Preliminaries

Let $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ be a dataset of n image $\mathbf{x}_i \in \mathbb{R}^{c\times d}$ and one-hot label map $\mathbf{y}_i \in \{0,1\}^{k\times d}$ pairs, with number of channels c, height times width $hw = d$, and categories k. We denote $\mathrm{softmax}_k(\cdot)$ as the row-wise softmax applied after reshaping the input from $\mathbb{R}^{kd}$ to $\mathbb{R}^{k\times d}$. To avoid cluttered notation, we may use lowercase symbols to denote both random variables and their realisations when context permits.

Stochastic Segmentation Networks. Stochastic Segmentation Networks (SSNs) [55] model joint distributions over label maps to generate spatially coherent segmentations. Pixel-wise dependencies are modelled by placing a low-rank multivariate Gaussian distribution over the logit space, and marginalising[1] the logits $\boldsymbol{\eta} \in \mathbb{R}^{kd}$ to compute likelihoods:

$$
\begin{aligned}
p(\mathbf{y} \mid \mathbf{x}) &= \int p(\mathbf{y} \mid \boldsymbol{\eta}) p(\boldsymbol{\eta} \mid \mathbf{x}) \, \mathrm{d}\boldsymbol{\eta}, \\
p(\boldsymbol{\eta} \mid \mathbf{x}) &= \mathcal{N}(\boldsymbol{\eta}; \boldsymbol{\mu}(\mathbf{x}), \boldsymbol{\Sigma}(\mathbf{x})), \\
p(\mathbf{y} \mid \boldsymbol{\eta}) &= \mathrm{Categorical}(\mathbf{y}; \mathrm{softmax}_k(\boldsymbol{\eta})), \qquad (1)
\end{aligned}
$$

[1] A Monte Carlo estimator of this (intractable) integral is typically used.

where $\boldsymbol{\mu}(\mathbf{x}) \in \mathbb{R}^{kd}$ and $\boldsymbol{\Sigma}(\mathbf{x}) \in \mathbb{R}^{kd \times kd}$ are predicted by a neural network given an input $\mathbf{x}$. Dependencies in logit space manifest in pixel space through the conditional dependence of $\mathbf{y}$ on $\boldsymbol{\eta}$. Note that $\boldsymbol{\Sigma}(\mathbf{x})$ is not only spatial but also class-wise. Due to the large number of pixels involved, estimating $\boldsymbol{\Sigma}(\mathbf{x})$ is typically computationally infeasible, thus, Monteiro et al. [55] use a low-rank approximation of the form:

$$\boldsymbol{\Sigma}(\mathbf{x}) = \mathbf{D}(\mathbf{x}) + \mathbf{P}(\mathbf{x})\mathbf{P}(\mathbf{x})^\top, \tag{2}$$

where $\mathbf{D}(\mathbf{x}) \in \mathbb{R}_+^{kd \times kd}$ denotes the diagonal matrix containing pixel-wise (including class-wise) independent variances, whereas the covariance factor matrix specifying r as the rank of the approximation is denoted by $\mathbf{P}(\mathbf{x}) \in \mathbb{R}^{kd \times r}$.

Normalising Flows. Normalising Flow (NF) [20, 62, 68, 81] models construct a complex probability distribution p_X of a target variable X by applying a parameterised transformation $\phi : \mathcal{U} \to \mathcal{X}$ to a simple base distribution p_U. If the transformation $\mathbf{x} = \phi(\mathbf{u})$ is both invertible and differentiable (i.e. *diffeomorphic*), the density of the target variable is readily given by the change-of-variables formula:

$$p_X(\mathbf{x}) = p_U(\mathbf{u}) \left|\det \mathbf{J}_\phi(\mathbf{u})\right|^{-1}, \quad \mathbf{u} = \phi^{-1}(\mathbf{x}), \tag{3}$$

where $(\mathbf{J}_\phi(\mathbf{u}))_{ij} = \partial \phi_i / \partial u_j$ is the Jacobian matrix. The design space of transformations ϕ is often restricted to cases where the Jacobian determinant is efficient to compute. Autoregressive flows [40, 61] use a chain of invertible transformations $\phi_1 \circ \phi_2 \circ \cdots \circ \phi_T$, each given by an autoregressive model. Autoregressive flows have been used to increase the flexibility of the approximate posterior in VAEs [40, 85].

Continuous Normalising Flows. Continuous Normalising Flows (CNFs) [12] define a time-dependent (for time $t \in [0, 1]$) continuous flow mapping $\phi_t(\mathbf{x})$ from a simple base density $\mathbf{x}_0 \sim p_0$ to a desired data distribution $\mathbf{x}_1 \sim p_{\text{data}}$ governed by an ordinary differential equation (ODE):

$$\frac{\mathrm{d}\phi_t(\mathbf{x})}{\mathrm{d}t} = v_t(\phi_t(\mathbf{x}); \theta), \qquad \phi_0(\mathbf{x}) = \mathbf{x}_0, \tag{4}$$

where $v_t(\phi_t(\mathbf{x}); \theta)$ is a vector field parameterised by a deep neural network with parameters θ. A vector field v_t is said to generate a *probability density path* p_t that transports p_0 to $p_1 \approx p_{\text{data}}$ if its flow ϕ_t satisfies the continuous-time analogue of the change-of-variables formula in Equation 3. To sample from the model, noise is mapped to data by solving the following differential equation using an ODE solver:

$$\phi_1(\mathbf{x}) = \mathbf{x}_1 = \mathbf{x}_0 + \int_0^1 v_t(\phi_t(\mathbf{x}); \theta)\, \mathrm{d}t. \tag{5}$$

Flow Matching (FM) [2, 48, 49] provides a simulation-free way of training CNFs by regressing a velocity field u_t, inducing a desired probability path p_t. However, both p_t and u_t are generally unknown; there exist many p_t's which generate p_{data}, and we do not know the u_t that generates p_t. Lipman et al. [48] showed that a chosen p_t and corresponding u_t can be constructed by marginalising *conditional* probability paths and vector fields over p_{data}. A conditional probability path $p_t(\mathbf{x} \mid \mathbf{x}_1)$ is a time-dependent distribution that satisfies the following marginal constraints at the endpoints:

$$p_0(\mathbf{x} \mid \mathbf{x}_1) = p_0(\mathbf{x}), \quad p_1(\mathbf{x} \mid \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \tag{6}$$

The marginal probability path and vector field are given by:

$$\begin{aligned} p_t(\mathbf{x}) &= \mathbb{E}_{\mathbf{x}_1 \sim p_{\text{data}}}\left[p_t(\mathbf{x} \mid \mathbf{x}_1)\right] \\ u_t(\mathbf{x}) &= \mathbb{E}_{\mathbf{x}_1 \sim p_{\text{data}}}\left[u_t(\mathbf{x} \mid \mathbf{x}_1) \frac{p_t(\mathbf{x} \mid \mathbf{x}_1)}{p_t(\mathbf{x})}\right], \end{aligned} \tag{7}$$

where the *conditional* vector field $u_t(\mathbf{x} \mid \mathbf{x}_1)$ is defined by the time derivative $\mathrm{d}\phi_t/\mathrm{d}t$ of the chosen flow map ϕ_t, which transports samples from p_0 to $p_t(\mathbf{x} \mid \mathbf{x}_1)$. A common choice is to set the flow to $\phi_t(\mathbf{x}_0 \mid \mathbf{x}_1) = \sigma_t(\mathbf{x}_1)\mathbf{x}_0 + \mu_t(\mathbf{x}_1)$, where $p_t(\mathbf{x} \mid \mathbf{x}_1) = \mathcal{N}(\mathbf{x}; \mu_t(\mathbf{x}_1), \sigma_t^2(\mathbf{x}_1) I)$ is Gaussian.

Crucially, Lipman et al. [48] showed that if $u_t(\mathbf{x} \mid \mathbf{x}_1)$ generates $p_t(\mathbf{x} \mid \mathbf{x}_1)$ then $u_t(\mathbf{x})$ generates $p_t(\mathbf{x})$ and the following simple regression objective can be used to train a CNF that generates the marginal probability path $p_t(\mathbf{x})$:

$$\mathbb{E}_{t, p_{\text{data}}(\mathbf{x}_1), p_t(\mathbf{x} \mid \mathbf{x}_1)}\left[\left\|u_t(\mathbf{x} \mid \mathbf{x}_1) - v_t(\mathbf{x}; \theta)\right\|^2\right], \tag{8}$$

with $t \sim \mathcal{U}(0, 1)$, thus approximating the unknown data distribution $p_1 \approx p_{\text{data}}$ at time $t = 1$, as intended.

4. Theoretical Analysis: Effective Rank

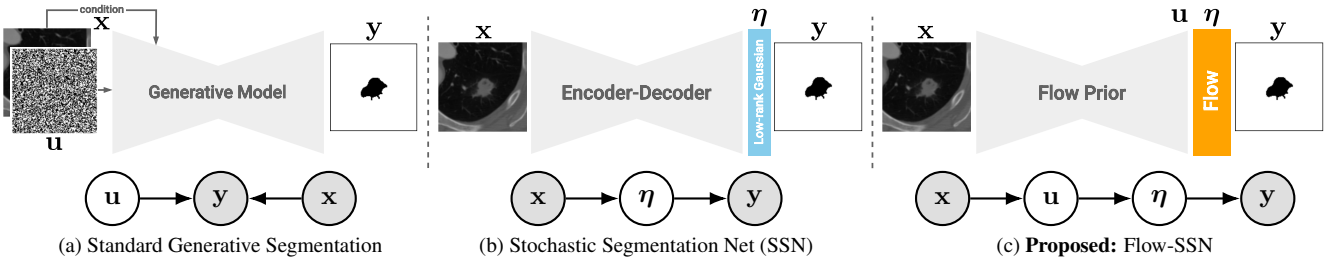
As outlined in Section 1, the low-rank assumption in SSNs is restrictive. Even if scaling the number of covariance factors (e.g. $r \gg 10$) were practical, it would still impose a Gaussian assumption on the pixel-space distribution. We now proceed with a theoretical analysis of the rank assumption in SSNs, to provide a more nuanced argument in favour of our flow-based approach. In short, we prove that the expected likelihood SSNs use results in a rank *increase* relative to the initially assumed rank, but the final effective rank only grows sublinearly w.r.t. the initial rank, limiting expressivity[2].

Lemma 4.1 (Rank Increase)**.** *Let the logits $\boldsymbol{\eta}$ be low-rank Gaussian distributed $\boldsymbol{\eta} \mid \mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}(\mathbf{x}), \boldsymbol{\Sigma}(\mathbf{x}))$, where the covariance $\boldsymbol{\Sigma}(\mathbf{x}) \in \mathbb{R}^{kd \times kd}$ has rank $\operatorname{rank}(\boldsymbol{\Sigma}(\mathbf{x})) = r$. Given that $\mathbf{y} = \operatorname{softmax}_k(\boldsymbol{\eta})$, the following holds:*

$$\operatorname{rank}(\operatorname{Cov}(\mathbf{y})) > r \iff r < d(k-1). \tag{9}$$

This result reveals that the low-rank approximation is not as restrictive as anticipated, as the non-linear pushforward by the softmax induces a rank *increase*. However, we now prove that the *effective* rank remains low, limiting expressivity.

[2] Proofs for all formal results are provided in Appendices A and B.



(a) Standard Generative Segmentation (b) Stochastic Segmentation Net (SSN) (c) **Proposed:** Flow-SSN

Figure 1. **Graphical models for stochastic segmentation**. **(a)** The typical setup, a generative model of label maps $\mathbf{y}$ conditioned on the image $\mathbf{x}$ (e.g. diffusion-based segmentation). **(b)** Stochastic segmentation network [55], a Markov chain with a low-rank Gaussian parameterisation of the logits $\boldsymbol{\eta}$, where $\mathbf{y} = \mathrm{softmax}(\boldsymbol{\eta})$. **(c)** A Flow-SSN (discrete or continuous-time), which consists of: (i) a parameterised conditional base distribution $p_{U|X}(\mathbf{u} \mid \mathbf{x}; \lambda)$ serving as an expressive flow *prior*; (ii) a lightweight flow $\phi : \mathcal{U} \to \mathcal{Y}$ to model pixel-wise dependencies.

Definition 4.2 (Effective Rank [73])**.** The effective rank $\mathrm{erank}(A) \in \mathbb{R}$ of a matrix $A \in \mathbb{R}^{d \times d}$ is given by:

$$\mathrm{erank}(A) = e^{H(p)}, \quad H(p) = -\sum_{i=1}^{d} p_i \log p_i, \tag{10}$$

where $H(p)$ is the Shannon entropy of the singular value distribution: $p_i = \sigma_i / \sum_{j=1}^{d} \sigma_j$, for $i \in \{1, \dots, d\}$, with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d \geq 0$ denoting the singular values of A.

Remark 4.3. Intuitively, the effective rank represents the average number of significant dimensions in a matrix's range.

Theorem 4.4 (Sublinear Growth of the Effective Rank)**.** *Given a low-rank Gaussian covariance matrix* $\boldsymbol{\Sigma}(\mathbf{x}) \in \mathbb{R}^{kd \times kd}$ *with initial rank* $\mathrm{rank}(\boldsymbol{\Sigma}(\mathbf{x})) = r < d(k-1)$*. The increase in the effective rank* $\mathrm{erank}(\mathrm{Cov}(\mathbf{y}))$*, in the sense of Lemma 4.1, grows sublinearly w.r.t.* r*.*

Theorem 4.4 shows that despite the induced rank increase as per Lemma 4.1, the final effective rank $\mathrm{erank}(\mathrm{Cov}(\mathbf{y}))$ only grows sublinearly w.r.t the initial rank r. Thus, the low-rank assumption is still highly restrictive for high-dimensional, pixel-wise covariances. This result may be of independent interest to other low-rank approximation techniques [32, 91].

5. Flow Stochastic Segmentation Networks

Motivated by the theoretical analysis in Section 4, we present Flow Stochastic Segmentation Networks (Flow-SSNs). Unlike standard SSNs, Flow-SSNs can estimate arbitrarily high-rank pixel-wise covariances without needing to assume the rank apriori or store distributional parameters. We begin our exposition by: (§5.1) designing *discrete-time* flows for learning pixel-wise covariances from an autoregressive perspective, then (§5.2) develop a generalisation of the approach to modern *continuous-time* flows, which admit free-form Jacobians. Flow-SSNs are also significantly more efficient to sample from than other diffusion-based segmentation models, as the majority of the model capacity is allocated to learning a flow's prior (normally fixed), while the flow network is lightweight, thereby reducing sampling cost substantially.

5.1. Discrete-Time Autoregressive Flow-SSNs

The motivation for using flows to model pixel-wise covariances in stochastic segmentation is simple. Since pixel-wise Gaussian covariances only represent linear dependencies between components, a *linear* autoregressive flow model is sufficient to transform a Gaussian distributed random variable with diagonal covariance into one with *full* covariance.

Proposition 5.1 (Full Covariance Flow Transformation)**.** *Let* $\mathbf{u} = (u_1, u_2, \dots, u_d)^\top$ *be a Gaussian distributed random vector with diagonal covariance* $\mathbf{u} \sim \mathcal{N}(\boldsymbol{\mu}, \mathrm{diag}(\boldsymbol{\sigma}^2))$*. A linear autoregressive model is sufficient to transform* $\mathbf{u}$ *into a new variable* $\boldsymbol{\eta} \in \mathbb{R}^d$ *with full covariance* $\boldsymbol{\Sigma} \in \mathbb{R}^{d \times d}$*.*

This result underpins our key model proposal, which consists of the following two components: (i) learn an expressive, but pixel-wise independent, flow base distribution conditional on $\mathbf{x}$ to act as an 'initial guess' logit distribution; (ii) use a lightweight autoregressive flow to model logit-space dependencies, thereby inducing *full* covariance structure as per Proposition 5.1, and refining the initial guess. Concretely, a Flow-SSN consists of the following two components:

(i) A conditional base distribution $p_{U|X}$, parameterised by a neural encoder-decoder $f_\lambda : \mathbb{R}^{c \times d} \to \mathbb{R}^{kd} \times \mathbb{R}^{kd}$:

$$p_{U|X}(\mathbf{u} \mid \mathbf{x}; \lambda) = \mathcal{N}\left(\mathbf{u}; \boldsymbol{\mu}(\mathbf{x}), \mathrm{diag}(\boldsymbol{\sigma}^2(\mathbf{x}))\right); \tag{11}$$

(ii) A lightweight autoregressive flow $\phi : \mathbb{R}^{kd} \to \mathbb{R}^{kd}$:

$$\forall i \; : \; \eta_i = \phi_i(\mathbf{u}_{\leq i}; \theta), \quad \mathbf{u}|\mathbf{x} \sim p_{U|X}. \tag{12}$$

The likelihood $p(\mathbf{y} \mid \mathbf{x})$ of a Flow-SSN can be obtained by marginalising the logit variables $\boldsymbol{\eta}$ similar to an SSN:

$$\begin{aligned} p(\mathbf{y} \mid \mathbf{x}) &= \int p(\mathbf{y} \mid \boldsymbol{\eta}) p(\boldsymbol{\eta} \mid \mathbf{x}; \lambda, \theta) \, \mathrm{d}\boldsymbol{\eta}, \\ p(\boldsymbol{\eta} \mid \mathbf{x}; \lambda, \theta) &= p_{U|X}(\mathbf{u} \mid \mathbf{x}; \lambda) \left|\det \mathbf{J}_\phi(\mathbf{u})\right|^{-1}, \\ p(\mathbf{y} \mid \boldsymbol{\eta}) &= \mathrm{Categorical}(\mathbf{y}; \mathrm{softmax}_k(\boldsymbol{\eta})), \end{aligned} \tag{13}$$

but $p(\boldsymbol{\eta} \mid \mathbf{x}; \lambda, \theta)$ is now more expressive than the low-rank Gaussian in SSNs, as it can model *full* covariance structure.

5.1.1. Designing a Flow & Objective

In this section, we explore the design space of autoregressive Flow-SSNs. Affine autoregressive flows are of the form $\eta_i = \phi_{\mu_i}(\boldsymbol{\eta}_{<i}) + \phi_{\sigma_i}(\boldsymbol{\eta}_{<i})u_i$, and have a tractable, lower triangular Jacobian: $\partial u_i / \partial \eta_j = 0, \forall j > i$. Using a Masked Autoregressive Flow (MAF) [61] for modelling $p(\boldsymbol{\eta} \mid \mathbf{x})$ is not ideal, as it requires slow, pixel-wise sequential sampling. Conversely, Inverse Autoregressive Flows (IAFs) [40] are fast to sample from, but require pixel-wise sequential scoring[3]. Crucially, IAFs can still score their *own* samples efficiently, as intermediate outputs can be cached.

This important fact opens up multiple design options for building discrete-time autoregressive Flow-SSNs, some of which we outline next and detail further in Appendix B.

Inverse Autoregressive Flow-SSN. A simple approach is to choose an IAF, and use a Monte Carlo estimator of the categorical likelihood in Eq. (13) analogous to standard SSNs:

$$\max_{\lambda,\theta} \mathbb{E}_{\mathbf{u}\sim p_{U|X}(\mathbf{u}|\mathbf{x};\lambda)} \left[\log p(\mathbf{y} \mid \boldsymbol{\eta} = \phi(\mathbf{u};\theta))\right]. \tag{14}$$

Dual Flow-SSN. A *dual* Flow-SSN comprised of an IAF $p^{\text{IAF}}(\boldsymbol{\eta} \mid \mathbf{x};\lambda,\theta)$ and an MAF $p^{\text{MAF}}(\boldsymbol{\eta} \mid \mathbf{x};\hat{\lambda},\hat{\theta})$ can be trained concurrently by maximising: $\log p(\mathbf{y} \mid \mathbf{x}) \geq$

$$\mathbb{E}_{\boldsymbol{\eta}\sim p^{\text{IAF}}(\boldsymbol{\eta}|\mathbf{x};\lambda,\theta)} \left[\log p(\mathbf{y} \mid \boldsymbol{\eta})\right] - D_{\text{KL}}\left(p^{\text{IAF}} \parallel p^{\text{MAF}}\right).$$

If we choose p^{MAF} as improper uniform: $\forall \boldsymbol{\eta}, p(\boldsymbol{\eta}) = \text{const}$, then we can avoid training the MAF by optimising:

$$\mathbb{E}_{\boldsymbol{\eta}\sim p^{\text{IAF}}(\boldsymbol{\eta}|\mathbf{x};\lambda,\theta)} \left[\log p(\mathbf{y} \mid \boldsymbol{\eta})\right] + \beta H(p^{\text{IAF}}), \tag{15}$$

where setting the hyperparameter $\beta > 0$ helps prevent p^{IAF} from collapsing to a deterministic model.

5.2. Continuous-Time Flow-SSNs

Relaxing the autoregressive structure of discrete-time Flow-SSNs induces a more expressive *free-form* Jacobian, but it complicates the computation of its determinant, as it is no longer simply the product of its diagonal elements. This calls for adapting continuous-time flows [2, 12, 48, 49] to build Flow-SSNs, as they can be trained efficiently via FM, admit free-form Jacobians, and can therefore model arbitrary pixel-wise covariances in stochastic segmentation tasks.

Interpolation Path. Continuous-time Flow-SSNs share the same design principle as their discrete-time counterparts, comprising: (i) an expressive conditional base distribution; (ii) a lightweight flow to model pixel-wise dependencies. However, the flow ϕ_t is now a continuous-time mapping from the conditional base distribution $\mathbf{u}|\mathbf{x} \sim p_{t=0} = p_{U|X}$ to the label data distribution $\mathbf{y} \sim p_{t=1} = p_{\text{data}}$, and it can be defined as a simple deterministic interpolation path:

$$\mathbf{y}_t = (1-t)\mathbf{u} + t\mathbf{y} \implies \mathrm{d}\mathbf{y}_t = (\mathbf{y} - \mathbf{u})\,\mathrm{d}t. \tag{16}$$

[3] As per Figure 2, the inverse transform of an affine autoregressive flow $\mathbf{u} = (\boldsymbol{\eta} - \boldsymbol{\mu}(\boldsymbol{\eta}))/\boldsymbol{\sigma}(\boldsymbol{\eta})$ is parallelisable since $u_i \perp\!\!\!\perp u_{j\neq i} \mid \{\eta_i, \mu_i, \sigma_i\}$.

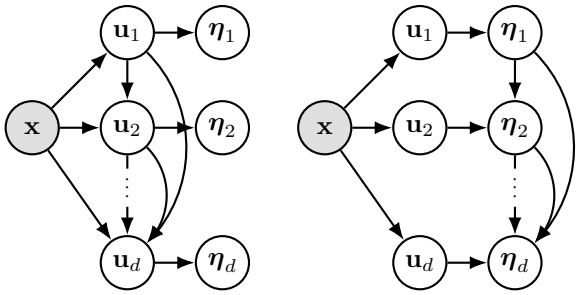


Figure 2. **Graphical models of autoregressive Flow-SSNs**. *Left*: inverse autoregressive; *Right*: masked autoregressive. The target variable $\mathbf{y}$ is omitted here for simplicity, noting that the logits $\boldsymbol{\eta} \rightarrow \mathbf{y}$ in all cases, e.g. via a deterministic transform $\mathbf{y} = \text{softmax}_k(\boldsymbol{\eta})$.

Importantly, the so-called *Markovian projection* $\mathcal{M}(\cdot)$ [29] of this type of ODE has been previously shown [65, 78] to preserve the marginals p_t for all time points $t \in [0, 1]$:

$$\mathrm{d}\mathbf{y}_t^\star = \mathcal{M}\left(\mathbf{y} - \mathbf{u}\right)\mathrm{d}t = \left(\mathbb{E}[\mathbf{y} \mid \mathbf{y}_t] - \mathbf{u}\right)\mathrm{d}t. \tag{17}$$

Therefore, in practice, we require a model $p(\cdot;\theta)$ to approximate the conditional expectation $\mathbb{E}[\mathbf{y} \mid \mathbf{y}_t]$, which we propose to parameterise using a *much smaller* neural network compared to the one used for learning the base distribution $p_{U|X}$ (i.e. prior). This makes sampling (ODE solving) *significantly* cheaper compared to typical generative segmentation models, where *all* the model parameters are dedicated to learning the score/velocity field [3, 66, 89, 92]. Further, one could then leverage a large foundation model as the prior.

Categorical Likelihood. Since $\mathbf{y}$ is a one-hot map, we have:

$$\begin{aligned}\mathbb{E}[\mathbf{y} \mid \mathbf{y}_t] &= \sum_{\mathbf{y}\in\{0,1\}^{k\times d}} \mathbf{y} \cdot \text{Categorical}(\mathbf{y}; \text{softmax}(\boldsymbol{\eta})) \\ &\approx \text{softmax}(\boldsymbol{\eta}(\phi_t(\mathbf{u} \mid \mathbf{y});\theta)),\end{aligned} \tag{18}$$

where $\phi_t(\mathbf{u} \mid \mathbf{y}) = \mathbf{y}_t = (1-t)\mathbf{u} + t\mathbf{y}$, and $\boldsymbol{\eta}(\cdot;\theta)$ is a neural network. Thus, like discrete-time Flow-SSNs (cf. Eq. (14)), we train using an expected categorical likelihood:

$$\max_{\lambda,\theta} \mathbb{E}_{\mathbf{u}\sim p_{U|X}(\mathbf{u}|\mathbf{x};\lambda)} \left[\int_0^1 \log p(\mathbf{y} \mid \mathbf{y}_t;\theta)\,\mathrm{d}t\right], \tag{19}$$

where $(\mathbf{x}, \mathbf{y}) \sim p_{\text{data}}(\mathbf{x}, \mathbf{y})$, and we now have $t \sim \mathcal{U}(0, 1)$. This objective differs from the standard FM objective and can be seen as a special case of variational FM [22]. However, the motivation and derivations presented here are distinct, as they are a natural consequence of infinite-depth Flow-SSNs.

Priors. Alternative priors for continuous-time Flow-SSNs can be specified by, e.g., a pushforward of the base distribution $f_{\#}p_{U|X}$, then defining the interpolant $\mathrm{d}\mathbf{y}_t = (\mathbf{y} - \boldsymbol{\eta})\mathrm{d}t$. For instance, if we choose $\boldsymbol{\eta} = f(\mathbf{u})$ as the log-softmax function, then $f_{\#}p_{U|X}$ is log-logistic normal. Another promising avenue is to consider mixture distributions (e.g. Gaussian) and/or leverage large foundation models as flexible priors.

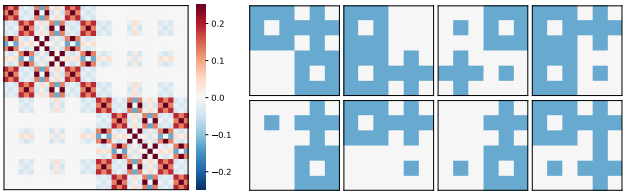


Figure 3. **The *MarkovShapes* dataset**. (*Left*) Ground truth pixel covariance matrix, rank r_{true}=12. (*Right*) Random data samples.

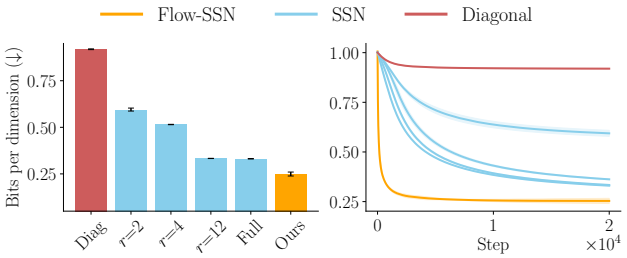
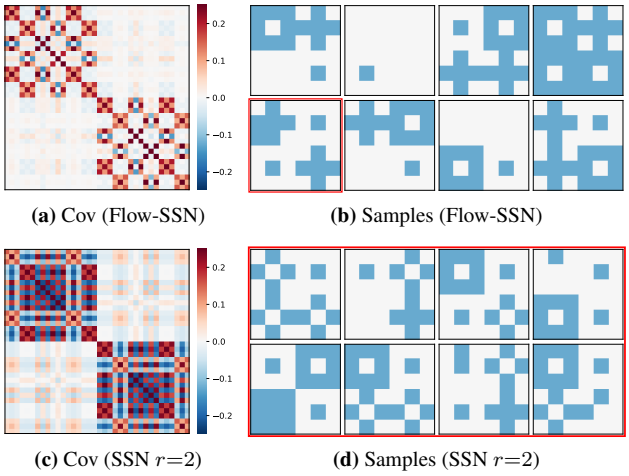


Figure 4. Bits per dimension (BPD) results on *MarkovShapes*.



(a) Cov (Flow-SSN) **(b)** Samples (Flow-SSN)

(c) Cov (SSN r=2) **(d)** Samples (SSN r=2)

Figure 5. **Comparing learnt covariances on *MarkovShapes***. (*Top*) Flow-SSNs make no rank assumptions and approximate the ground truth covariance well. (*Bottom*) The low-rank approximation causes sampling errors, even under a mild underspecification ratio, r=2 relative to r_{true}=12. Sampling errors (hallucinated shapes not faithful to the true covariance structure) are indicated with red boxes.

6. Experiments

6.1. Toy Problem: MarkovShapes

In this experiment, we introduce a synthetic dataset, *MarkovShapes*, where we have full control of the rank of the pixel-space covariance. Comparing Flow-SSN with the low-rank SSN model [55], *MarkovShapes* reveals how the SSN fails when the assumed rank is underspecified and demonstrates how Flow-SSN overcomes this shortcoming.

MarkovShapes consists of images composed of 3 possible shapes: '*square*' (□), '*plus*' (✚) and '*dot*'(▪). Each image quadrant is either filled with a shape or left empty (∅) at random. The data-generating process is a Markov chain, with states corresponding to shapes and the transitions between quadrants governed by the doubly stochastic matrix $\mathbf{T}$:

$$\mathbf{T} = \begin{array}{c} \\ \varnothing \\ \square \\ \boxplus \\ \blacksquare \end{array} \begin{array}{c} \begin{array}{cccc} \varnothing & \square & \boxplus & \blacksquare \end{array} \\ \begin{bmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 3/40 & 27/80 & 27/80 \\ 1/4 & 27/80 & 3/40 & 27/80 \\ 1/4 & 27/80 & 27/80 & 3/40 \end{bmatrix} \end{array}, \tag{20}$$

where $\mathbf{T}_{ij} = P(X_{t+1} = j \mid X_t = i)$ is the probability of transitioning from shape i to j within a particular image. Figure 3 shows the induced pixel covariance matrix, its empirically calculated true rank r_{true}, and random samples.

We adapt the SSN from the toy problem of Monteiro et al. [55], training four variants from rank 2 to full-rank on *MarkovShapes*. We implement and train a discrete-time autoregressive Flow-SSN with the objective in Eq. (14). We choose a single linear layer with MADE-style masking [26] for the autoregressive flow model. In all cases, we train for 20K steps using the Adam optimiser with 10^{-3} learning rate, batch size 32, and 512 MC samples. Figure 4 plots the performance of Flow-SSN against the baseline SSN, showing how Flow-SSN outperforms all SSN variants. Notably, Flow-SSN converges faster *and* achieves a better final result than even the full-rank SSN. In Figure 5, we show how samples from Flow-SSN faithfully represent each of the underlying shapes (i.e. □, ✚, and ▪). In contrast, the rank 2 SSN introduces sampling errors, hallucinating nonexistent shapes due to poorly modelling the true covariance structure.

Rank Underspecification Ratio. The underspecification ratio used for the SSN models on *MarkovShapes* (most extreme is r=2 : r_{true}=12) is mild compared to more complex high-dimensional real-world data, where $r \ll r_{\text{true}}$. Thus, the low-rank assumption of SSNs, typically r=10, is likely even more punishing in real-world settings. As shown in the next experiment, simply increasing the assumed rank for real-world data collapses the SSN to a deterministic model.

6.2. Lung Nodule Segmentation

The LIDC-IDRI dataset [4] is a standard benchmark for evaluating stochastic segmentation models, with multiple ground truth label maps per image reflecting the inherent variability among medical experts. LIDC contains 1018 lung CT scans, with lung nodule annotation masks provided by 4 radiologists (from a pool of 12). We use the preprocessing from Baumgartner et al. [6], Kohl et al. [43], where 128×128 patches are extracted such that each patch is centred on a nodule. The process yields 15,096 slices with 4 segmentations

Table 1. **Quantitative results on LIDC-IDRI**. Flow-SSN achieves SOTA performance with fewer params. (Δ/∞ denote discrete/continuous time variants). Results with (†) are from Zhang et al. [96]. $D^2_{\text{GED}}(M)$ denotes $16<M\leq100$ MC samples used. More baselines in App. E.

	LIDC-IDRI (128×128)					
METHOD	$D^2_{\text{GED}}(16)\downarrow$	$D^2_{\text{GED}}(M)\downarrow$	Diversity ↑	Dice ↑	HM-IoU ↑	#Param
UNet [72]†	-	0.676±.000	-	0.519±.004	0.463±.000	9M
ProbUNet [43]	0.287±N/A	0.252±.004	0.469±.003	0.390±.004	0.500±.030	18M
cFlow [76]†	-	0.225±.002	0.523±.010	0.449±.000	0.584±.000	N/A
PHiSeg [6]	-	0.225±.004	0.496±.003	0.486±.010	0.595±.00†	63M
SSN [55]	-	0.225±.002	0.609±.002	0.436±.004	0.555±.01†	41M
P²SAM [33]	0.218±N/A	0.216±N/A	-	-	0.679±N/A	N/A
SSN++ (ours)	0.241±.001	0.212±.001	0.575±.005	0.471±.003	-	20M
JProbUNet [96]	-	0.206±.000	0.475±.010	0.511±.010	0.647±.010	N/A
MoSE [25]	0.218±.003	0.189±.002	-	-	0.624±.004	42M
Flow-SSN$_\Delta$: {IAF, 1-step}	0.240±.002	0.212±.001	0.598±.000	0.468±.002	**0.879**±.000	14M
Flow-SSN$_\infty$: {Dopri5, tol=1e-6}	0.209±.002	0.182±.001	0.521±.005	0.610±.003	0.872±.000	14M
Flow-SSN$_\infty$: {Euler, T=50}	0.210±.002	0.182±.000	0.518±.006	0.611±.003	0.873±.000	14M
Flow-SSN$_\infty$: {Euler, T=250}	**0.207**±.000	**0.181**±.000	0.520±.006	**0.611**±.007	0.873±.001	14M

each, with a $60/20/20$ train/valid/test split. As in previous work, we measure performance using Generalised Energy Distance (GED), Dice, and Hungarian-Matched Intersection over Union (HM-IoU) [44, 66, 92]. Our architecture is a streamlined version of the Dhariwal and Nichol [19]'s UNet to parameterise both the prior and the continuous-time flow. We use a *single* autoregressive Transformer layer to parameterise our discrete-time Flow-SSN; the IAF variant trained using Eq. (14). For more details/results, see Appendix D/E.

Table 1 reports our results. Our baseline SSN (SSN++) outperforms the original [55], and the Flow-SSN achieves state-of-the-art performance in all metrics using fewer parameters[4]. Fig. 6 shows ablation results for learning the base distribution (i.e. prior) vs holding it fixed (as typically done). We observe a *significant* reduction in inference time without sacrificing performance, thanks to using a small network for the flow and allocating most of the model capacity to the prior (150K vs 14M params). Flow-SSN is $\simeq10\times$ more efficient than CCDM [92] (cf. App. E), and can perform competitively with just 10 ODE solver steps (c.f. Fig. 7).

6.3. Optical Cup Segmentation

REFUGE2 [23] is a publicly available benchmark dataset for optic disk and optic cup segmentation. Each fundus image in the dataset has multiple associated ground-truth label maps. Specifically, it includes annotations from 7 different independent ophthalmologists, each with an average of 8 years of experience. It contains a total of 1200 images, 400 for training, validation, and testing, respectively. Segmentation of the optic cup is inherently more variable than segmentation of the optic disk [23], therefore, we only consider the former in this work. As before, we measure performance using GED, Dice,

[4]We note that diversity is only relevant contextually, as high diversity can be trivially achieved with random noise as a model.

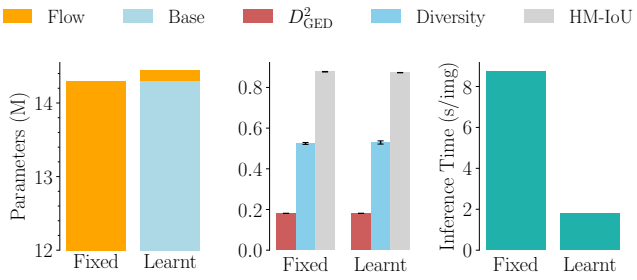


Figure 6. **Comparing learnt vs fixed priors in Flow-SSNs**. We observe a $5\times$ reduction in inference time without sacrificing performance. The flow network used in the learnt prior setup is around $100\times$ smaller than the fixed prior baseline, making ODE solving much cheaper. Note that s/img here includes inferring 100 MC samples per image, effectively performing 100 forward passes.

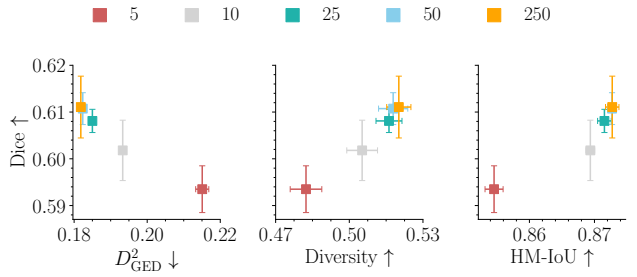


Figure 7. **Ablation study of the number of ODE solving steps**. Results (LIDC-IDRI) obtained using the Euler method. Flow-SSNs can perform competitively with as few as T=10 ODE solver steps.

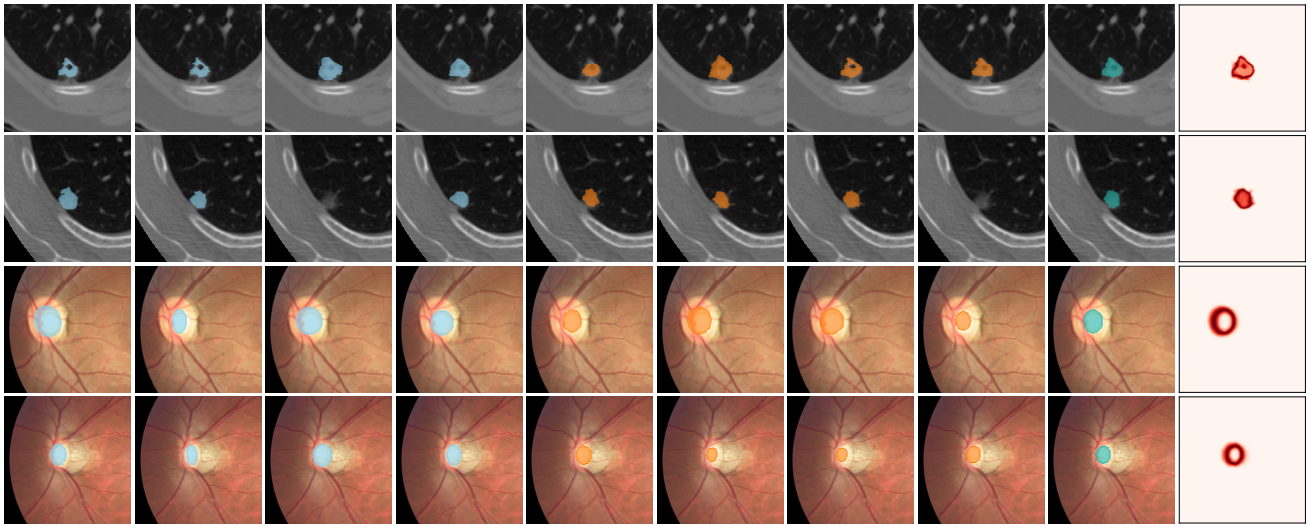


Figure 8. **Qualitative results on LIDC-IDRI (*Rows 1, 2*) and REFUGE-MultiRater (*Rows 3, 4*) using Flow-SSN**. (*Cols. 1-4*) Multiple ground-truth expert segmentations; (*Cols. 5-8*) Non-cherry-picked model samples; (*Cols. 9, 10*) Mean prediction and pixel uncertainty map.

Table 2. **Stochastic segmentation on REFUGE-MultiRater**. We set *new* benchmarks for D^2_{GED}, Diversity and HM-IoU. We use Δ and ∞ to denote discrete and continuous-time Flow-SSN variants.

		REFUGE-MultiRater (256×256)		
METHOD	M	$D^2_{\text{GED}} \downarrow$	Diversity ↑	HM-IoU ↑
Flow-SSN$_\Delta$	16	0.116±.007	0.441±.012	0.766±.006
	100	0.089±.004	0.462±.013	0.851±.001
	512	**0.081**±N/A	0.447±N/A	**0.881**±N/A
Flow-SSN$_\infty$	16	0.112±.003	0.424±.004	0.751±.003
	100	**0.089**±.001	0.453±.020	**0.832**±.004

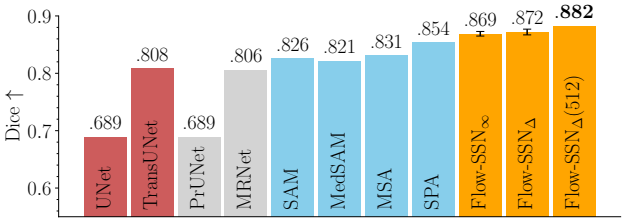


Figure 9. **Optical cup segmentation on REFUGE-MultiRater**. Baselines are from Zhu et al. [99]. We observe impressive Dice performance using modestly-sized Flow-SSNs with only 15M params.

and HM-IoU. For training, we resize the images to 256×256 to match the output size used by Zhu et al. [99] and enable fair comparisons with their reported Dice baselines. Namely, TransUNet [10], MRNet [10], SAM [42], MedSAM [51] and MSA [97]. For training details, please refer to Appendix D, and for extra ablation results see Appendix E. As shown in Fig. 9, Flow-SSNs outperform all baselines by a considerable margin using only 15M parameters. Table 2 provides *new* stochastic segmentation benchmark results, featuring both discrete and continuous-time Flow-SSN variants.

Surprisingly, we find that a discrete-time autoregressive Flow-SSN (a single-step IAF trained as per Eq. (14)) outperforms the continuous-time one on this dataset. We expect continuous-time Flow-SSNs to outperform shallow discrete-time ones in general, but this result encourages further exploration into this model class, as the discrete-time Flow-SSN is ≈200× faster to sample from than the continuous-time one. For this reason, we were able to push the number of MC samples used for evaluation up to M=512 and observed further significant gains in performance on all metrics.

7. Conclusion

We introduce the Flow Stochastic Segmentation Network (Flow-SSN), a generative segmentation model featuring both discrete-time autoregressive and modern continuous-time flow variants. By overcoming the constraints of low-rank parameterisations in standard SSNs, Flow-SSNs enable the estimation of arbitrarily high-rank pixel-wise covariances without requiring prior assumptions about rank or explicit storage of distributional parameters. Moreover, Flow-SSNs significantly improve sampling efficiency compared to standard diffusion-based segmentation models, thanks to a key architectural design that includes learning the base distribution (i.e. the prior) of the flow, which is typically fixed. Experimental results on standard real-world benchmarks demonstrate the efficacy of Flow-SSNs, achieving state-of-the-art performance, and highlighting their potential to advance stochastic segmentation in safety-critical applications with inherent ambiguities, such as medical imaging.

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