Change of Variables and Normalizing Flows

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Marc Peter Deisenroth

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Normalizing flows for density estimation

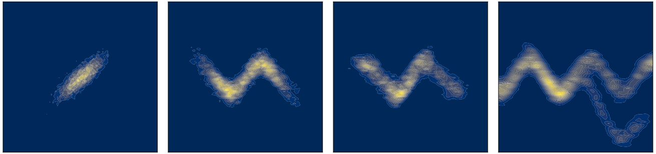

Figure: Generated with PyMC3 (Salvatier et al., 2016)

Key idea (Tabak & Turner, 2013; Rippel & Adams, 2013; Rezende & Mohamed, 2015)

Build complex distributions from simple distributions via a flow of successive (invertible) transformations

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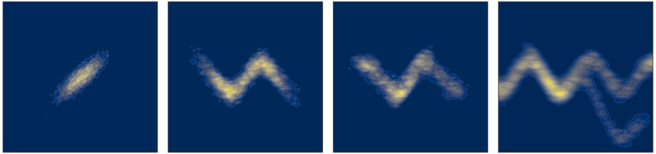

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Key idea
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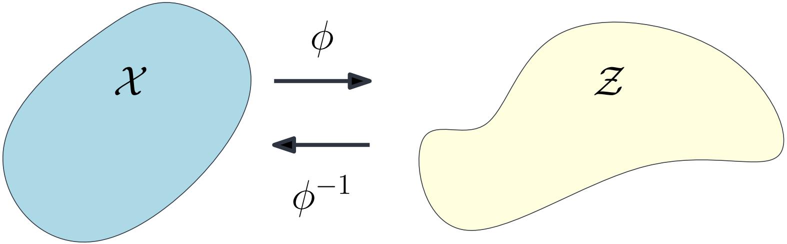
Build complex distributions from simple distributions via a flow of successive (invertible) transformations

Key ingredient: **Change-of-variables trick**

Change of Variables

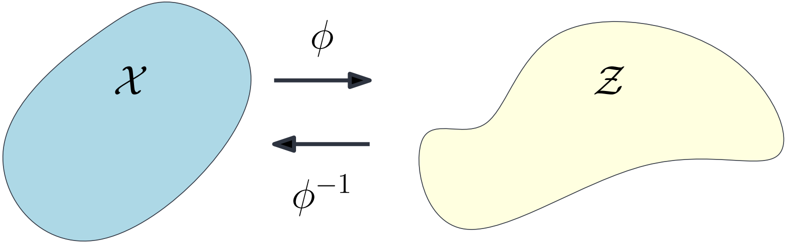
Change of variables: Key idea



Key idea

Transform random variable X into random variable Z using an invertible transformation ϕ, while keeping track of the change in distribution

Change of variables: Key idea

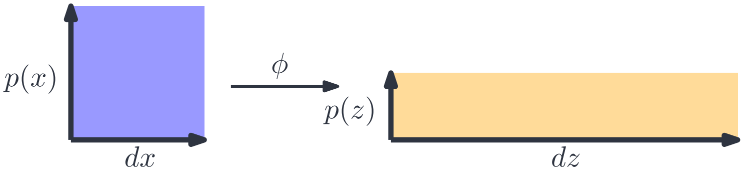


Key idea

Transform random variable X into random variable Z using an invertible transformation ϕ, while keeping track of the change in distribution

- Distribution p_X induces distribution p_Z via transformation ϕ
- Distribution p_Z induces distribution p_X via transformation ϕ^{-1}

Jacobian determinant



- Determinant of Jacobian

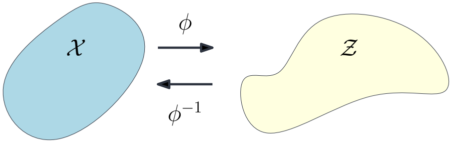
$$\left|\det\left(\frac{dz}{dx}\right)\right| = \left|\det\left(\frac{d\phi(x)}{dx}\right)\right|$$

tells us how much the domain dx is stretched to dz

How it works

- Constraint: volume preservation

$$\int_{\mathcal{X}} p_X(\boldsymbol{x}) d\boldsymbol{x} = 1 = \int_{\mathcal{Z}} p_Z(\boldsymbol{z}) d\boldsymbol{z}$$



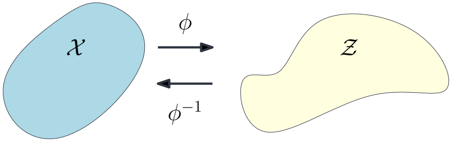
How it works

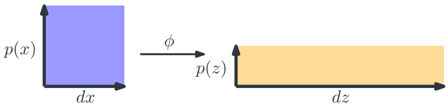
- Constraint: volume preservation

$$\int_{\mathcal{X}} p_X(\boldsymbol{x})d\boldsymbol{x} = 1 = \int_{\mathcal{Z}} p_Z(\boldsymbol{z})d\boldsymbol{z}$$

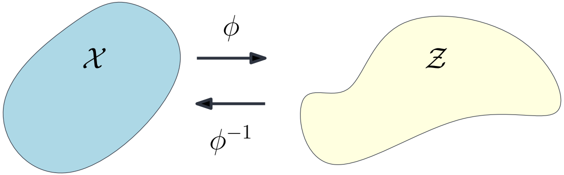
- Volume preservation: Rescale p_Z by the inverse of Jacobian determinant

$$p_Z(\boldsymbol{z}) = p_X(\boldsymbol{x}) \left| \det \left(\frac{d\phi(\boldsymbol{x})}{d\boldsymbol{x}} \right) \right|^{-1}$$





Considerations



$$p_Z(\boldsymbol{z}) = p_X(\boldsymbol{x}) \left| \det \left(\frac{d\phi(\boldsymbol{x})}{d\boldsymbol{x}} \right) \right|^{-1}$$

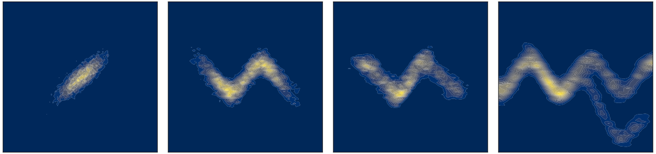
- Express target distribution p_Z in terms of known distribution p_X and the Jacobian determinant of an invertible mapping ϕ
- No need to invert ϕ explicitly
- Generate expressive distributions p_Z by simple p_X and flexible transformation ϕ

Applications

- Numerical integration (turn indefinite integrals into definite ones)
- Neural ODEs (E 2017, Chen et al., 2018)
- Learning in implicit generative models (e.g., GANs) and likelihood-free inference (e.g., ABC)
  (e.g., Mohamed & Lakshminarayanan, 2016; Sisson et al., 2007)
- **Normalizing flows** (Rezende & Mohamed, 2015)

Normalizing Flows

Normalizing flows for density estimation



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Key idea
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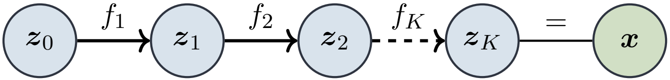
Build complex distributions from simple distributions via a flow of successive (invertible) transformations

How it works



$$z_0 \xrightarrow{f_1} z_1 \xrightarrow{f_2} z_2 \xrightarrow{f_K} z_K = x$$

- Random variable $\boldsymbol{z}_0 \sim p_0$
- Simple base distribution p_0, e.g. $p_0 = \mathcal{N}(\mathbf{0}, \boldsymbol{I})$

How it works

$$\begin{tikzcd} \boldsymbol{z}_0 \arrow[r, "f_1"] & \boldsymbol{z}_1 \arrow[r, "f_2"] & \boldsymbol{z}_2 \arrow[r, dashed, "f_K"] & \boldsymbol{z}_K \arrow[r, dash, "="] & \boldsymbol{x} \end{tikzcd}$$

- Random variable $\boldsymbol{z}_0 \sim p_0$
- Simple base distribution p_0, e.g. $p_0 = \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
- Successive transformation of $\boldsymbol{z}_k$ via invertible transformations f_k:

$$\boldsymbol{z}_k = f_k(\boldsymbol{z}_{k-1})$$

- Observed data $\boldsymbol{x} = \boldsymbol{z}_K$ at the end of the chain

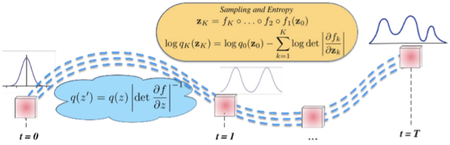
$$\boldsymbol{x} = \boldsymbol{z}_K = f_K \circ f_{K-1} \circ \cdots \circ f_1(\boldsymbol{z}_0)$$

Marginal distribution

$$\boldsymbol{z}_0 \xrightarrow{f_1} \boldsymbol{z}_1 \xrightarrow{f_2} \boldsymbol{z}_2 \overset{f_K}{\dashrightarrow} \boldsymbol{z}_K = \boldsymbol{x}$$

- Repeated application of **change-of-variables** trick

$$p(\boldsymbol{x}) = p(\boldsymbol{z}_K) = p(\boldsymbol{z}_0) \prod_{k=1}^{K} \left| \det \frac{df_k(\boldsymbol{z}_{k-1})}{d\boldsymbol{z}_{k-1}} \right|^{-1}$$



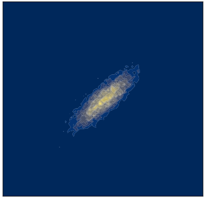
Distribution flows through a sequence of invertible transforms

Rezende and Mohamed, 2015

- Entropy

$$\log p(\boldsymbol{x}) = \log p(\boldsymbol{z}_K) = \log p(\boldsymbol{z}_0) - \sum_{k=1}^{K} \log \left| \det \left(\frac{df_k(\boldsymbol{z}_{k-1})}{d\boldsymbol{z}_{k-1}} \right) \right|$$

Illustration with PyMC3 (Salvatier et al., 2016)



1 planar flow

Figure: Generated using a PyMC3 tutorial (Salvatier et al., 2016)

- Repeated application of a planar flow $\boldsymbol{z}_k = f_k(\boldsymbol{z}_{k-1}) = \boldsymbol{z}_{k-1} + \boldsymbol{u}\sigma(\boldsymbol{w}^\top \boldsymbol{z}_{k-1} + b)$

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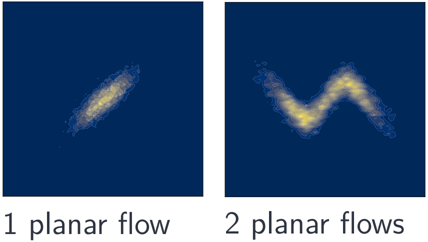

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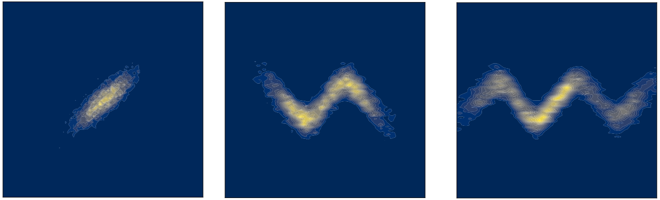

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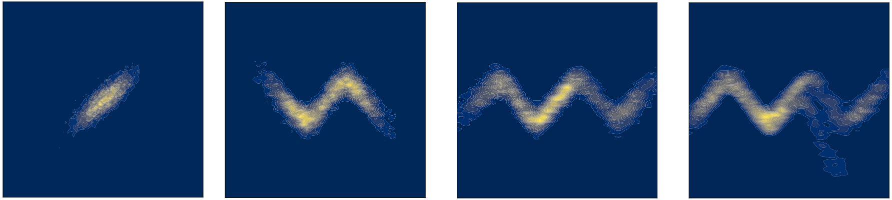

1 planar flow 2 planar flows 3 planar flows 7 planar flows

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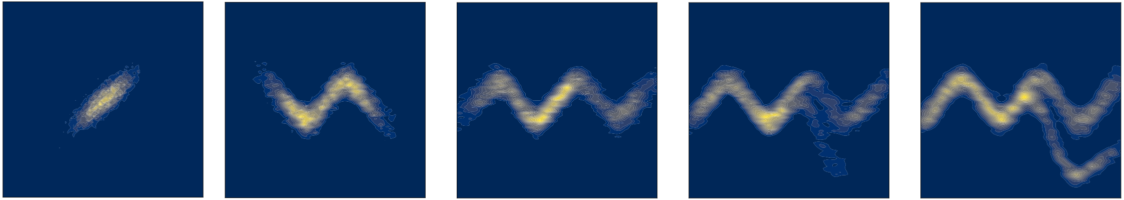

1 planar flow | 2 planar flows | 3 planar flows | 7 planar flows | 12 planar flows

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- Repeated application of a planar flow $\boldsymbol{z}_k = f_k(\boldsymbol{z}_{k-1}) = \boldsymbol{z}_{k-1} + \boldsymbol{u}\sigma(\boldsymbol{w}^\top \boldsymbol{z}_{k-1} + b)$

Computing expectations

$$\mathbb{E}_{p_X}[l(\boldsymbol{x})] = \mathbb{E}_{p_K}[l(\boldsymbol{z}_K)] = \mathbb{E}_{p_0}[l(f_K \circ \cdots \circ f_1(\boldsymbol{z}_0))]$$

Computing expectations

$$\mathbb{E}_{p_X}[l(\boldsymbol{x})] = \mathbb{E}_{p_K}[l(\boldsymbol{z}_K)] = \mathbb{E}_{p_0}[l(f_K \circ \cdots \circ f_1(\boldsymbol{z}_0))]$$

- Expectations w.r.t. p_K can be computed without explicitly knowing p_K or p_X
  - Sample $\boldsymbol{z}_0^{(s)} \sim p_0$
  - Push sample forward through sequence of deterministic transformations
  - ⏩ Valid sample $\boldsymbol{x}^{(s)} \sim p_X(\boldsymbol{x})$
- Monte-Carlo estimation to get expected value

Computational considerations

- Compute log-determinant of Jacobian
- Cheap (linear) if Jacobian is (block-)diagonal or triangular

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- Compute log-determinant of Jacobian
- Cheap (linear) if Jacobian is (block-)diagonal or triangular
- Require partial derivatives

$$\frac{\partial z_k^{(d)}}{\partial z_{k-1}^{(>d)}} = 0 \quad \blacktriangleright\!\!\blacktriangleright\!\!\blacktriangleright \quad \frac{d\boldsymbol{z}_k}{d\boldsymbol{z}_{k-1}} = \begin{bmatrix} \frac{\partial z_k^{(1)}}{\partial z_{k-1}^{(1)}} & \mathbf{0} & \dots & \mathbf{0} \\ \frac{\partial z_k^{(2)}}{\partial z_{k-1}^{(1)}} & \frac{\partial z_k^{(2)}}{\partial z_{k-1}^{(2)}} & \dots & \vdots \\ \vdots & & \ddots & \mathbf{0} \\ \frac{\partial z_k^{(D)}}{\partial z_{k-1}^{(1)}} & \dots & \dots & \frac{\partial z_k^{(D)}}{\partial z_{k-1}^{(D)}} \end{bmatrix} \in \mathbb{R}^{D \times D}.$$

Autoregressive flows

- High-level idea:

$$z_k^{(d)} = \phi(z_{k-1}^{(\leq d)})$$

Autoregressive flows

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- NICE (Dinh et al., 2014)
- Inverse autoregressive flow (Kingma et al., 2016)
- Real NVP (Dinh et al., 2017)
- Masked autoregressive flow (Papamakarios et al., 2017)
- Glow (Kingma & Dhariwal, 2018)
- (Block) neural autoregressive flows, spline flows, ... (e.g., Huang et al., 2018; de Cao et al., 2019; Durkan et al., 2019)

Application areas

- Variational inference in deep generative models (e.g., Rezende & Mohamed, 2015)
- Graph neural networks (Liu et al., 2019)
- Parallel WaveNet (van den Oord et al., 2018)

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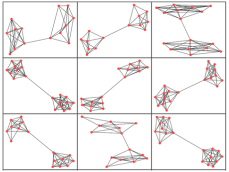
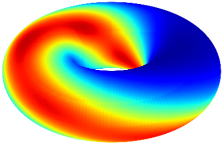
- Variational inference in deep generative models (e.g., Rezende & Mohamed, 2015)
- Graph neural networks (Liu et al., 2019)
- Parallel WaveNet (van den Oord et al., 2018)
- Continuous flows
  - Neural ODEs (e.g, E, 2017; Chen et al., 2018)
  - Flows on manifolds (e.g., Gemici et al., 2016; Rezende et al., 2020; Mathieu & Nickel, 2020)

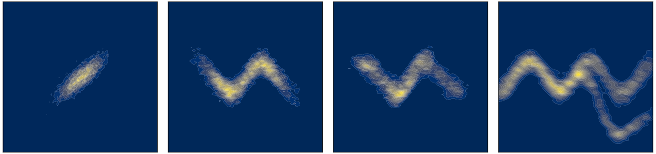


From Liu et al. (2019)



From Rezende et al. (2020)

Summary



- Normalizing flows provide a constructive way to generate rich distributions
- Key idea: Transform a simple distribution using a flow of successive (invertible) transformations
- Key ingredient: Change-of-variables trick
- Jacobians can be computed efficiently, if the transformations are defined appropriately
- Can be used as a generator and inference mechanism

References

Chen, T. Q., Rubanova, Y., Bettencourt, J., and Duvenaud, D. K. (2018). Neural Ordinary Differential Equations. In *Advances in Neural Information Processing Systems*.

De Cao, N., Aziz, W., and Titov, I. (2019). Block Neural Autoregressive Flow. In *Proceedings of the Conferene on Uncertainty in Artificial Intelligence*.

Dinh, L., Krueger, D., and Bengio, Y. (2014). NICE: Non-linear Independent Components Estimation. *arXiv:1410.8516*.

Dinh, L., Sohl-Dickstein, J., and Bengio, S. (2017). Density Estimation Using Real NVP. In *Proceedings of the International Conference on Learning Representation*.

Durkan, C., Bekasov, A., Murray, I., and Papamakarios, G. (2019). Neural Spline Flows. In *Advances in Neural Information Processing Systems*.

E, W. (2017). A Proposal on Machine Learning via Dynamical Systems. *Communications in Mathematics and Statistics*, 5(1):1–11.

References (cont.)

Gemici, M. C., Rezende, D. J., and Mohamed, S. (2016). Normalizing Flows on Riemannian Manifolds. *arXiv:1611.02304*.

Huang, C.-W., Krueger, D., Lacoste, A., and Courville, A. (2018). Neural Autoregressive Flows. In *Proceedings of the International Conference on Machine Learning*.

Kingma, D. P. and Dhariwal, P. (2018). Glow: Generative Flow with Invertible 1×1 Convolutions. In *Advances in Neural Information Processing Systems*.

Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., and Welling, M. (2016). Improved Variational Inference with Inverse Autoregressive Flow. In *Advances in Neural Information Procesing Systems*.

Kobyzev, I., Prince, S., and Brubaker, M. (2020). Normalizing Flows: An Introduction and Review of Current Methods. *IEEE Transactions on Pattern Analysis and Machine Intelligence*.

Liu, J., Kumar, A., Ba, J., Kiros, J., and Swersky, K. (2019). Graph Normalizing Flows. In *Advances in Neural Information Processing Systems*.

References (cont.)

Mathieu, E. and Nickel, M. (2020). Riemannian Continuous Normalizing Flows. *arXiv:2006.10605*.

Mohamed, S. and Lakshminarayanan, B. (2016). Learning in Implicit Generative Models. *arXiv:1610.03483*.

Oord, A., Li, Y., Babuschkin, I., Simonyan, K., Vinyals, O., Kavukcuoglu, K., Driessche, G., Lockhart, E., Cobo, L., Stimberg, F., Casagrande, N., Grewe, D., Noury, S., Dieleman, S., Elsen, E., Kalchbrenner, N., Zen, H., Graves, A., King, H., Walters, T., Belov, D., and Hassabis, D. (2018). Parallel WaveNet: Fast High-Fidelity Speech Synthesis. In *Proceedings of the International Conference on Machine Learning*.

Papamakarios, G., Nalisnick, E., Rezende, D. J., Mohamed, S., and Lakshminarayanan, B. (2019). Normalizing Flows for Probabilistic Modeling and Inference. *arXiv:1912.02762*.

Papamakarios, G., Pavlakou, T., and Murray, I. (2017). Masked Autoregressive Flow for Density Estimation. In *Advances in Neural Information Processing Systems*.

Rezende, D. J. and Mohamed, S. (2015). Variational Inference with Normalizing Flows. In *Proceedings of the International Conference on Machine Learning*.

References (cont.)

Rezende, D. J., Papamakarios, G., Racanière, S., Albergo, M. S., Kanwar, G., Shanahan, P. E., and Cranmer, K. (2020). Normalizing Flows on Tori and Spheres. In *Proceedings of the International Conference on Machine Learning*.

Rippel, O. and Adams, R. P. (2013). High-Dimensional Probability Estimation with Deep Density Models. *arXiv:1302.5125*.

Salvatier, J., Wiecki, T. V., and Fonnesbeck, C. (2016). Probabilistic Programming in Python using PyMC3. *PeerJ Computer Science*, 2:e55.

Sisson, S. A., Fan, Y., and Tanaka, M. M. (2007). Sequential Monte Carlo Without Likelihoods. *Proceedings of the National Academy of Sciences of the United States of America*, 104(6):1760–1765.

Tabak, E. G. and Turner, C. V. (2013). A Family of Nonparametric Density Estimation Algorithms. *Communications on Pure and Applied Mathematics*, 66(2):145–164.