Autoregressive and Invertible Models

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Outline

If training vanilla neural nets is optimization over functions, training recurrent nets is optimization over programs.

- Recurrent neural networks
  - General Idea
  - Gated Recurrent Unit
  - Pros and Cons
  - Applications
- Invertible Models
  - Overview
  - Real NVP
  - Extensions

Recurrent Neural Networks - General Idea

- Models series data by factorizing the joint probability

$$p(x_1, x_2, ..., x_n) = \prod_{k=1}^{n} p(x_k | x_1, ..., x_{k-1})$$

- Summarize the information from previous observations in a sufficient statistic, *h*

$$p(x_k | x_1, ..., x_{k-1}) = g_\theta(x_k | h_{k-1})$$

- Loss Function: Negative Log-Likelihood

$$-l(\theta) = -\sum_{k=1}^{n} \log g_\theta(x_k | h_{k-1})$$

Recurrent Neural Networks - General Idea

- Autoregressive: using data from previous observations to predict next observation
- *f* generates hidden and deterministic states *h* given inputs *x*
- *g* generates probability distribution (or mass) functions for next *x* given *h*
  - For discrete *x*, *g* contains a normalization by softmax
- h_0 must be initialized; it can be initialized by...
  - Sampling from some distribution
  - Learning it as an additional parameter
  - Using external information

$$p(x_k|x_1, ..., x_{k-1}) = g_\theta(x_k|h_{k-1})$$

$$h_k = f_\theta(x_k, h_{k-1})$$

Recurrent Neural Networks - General Idea

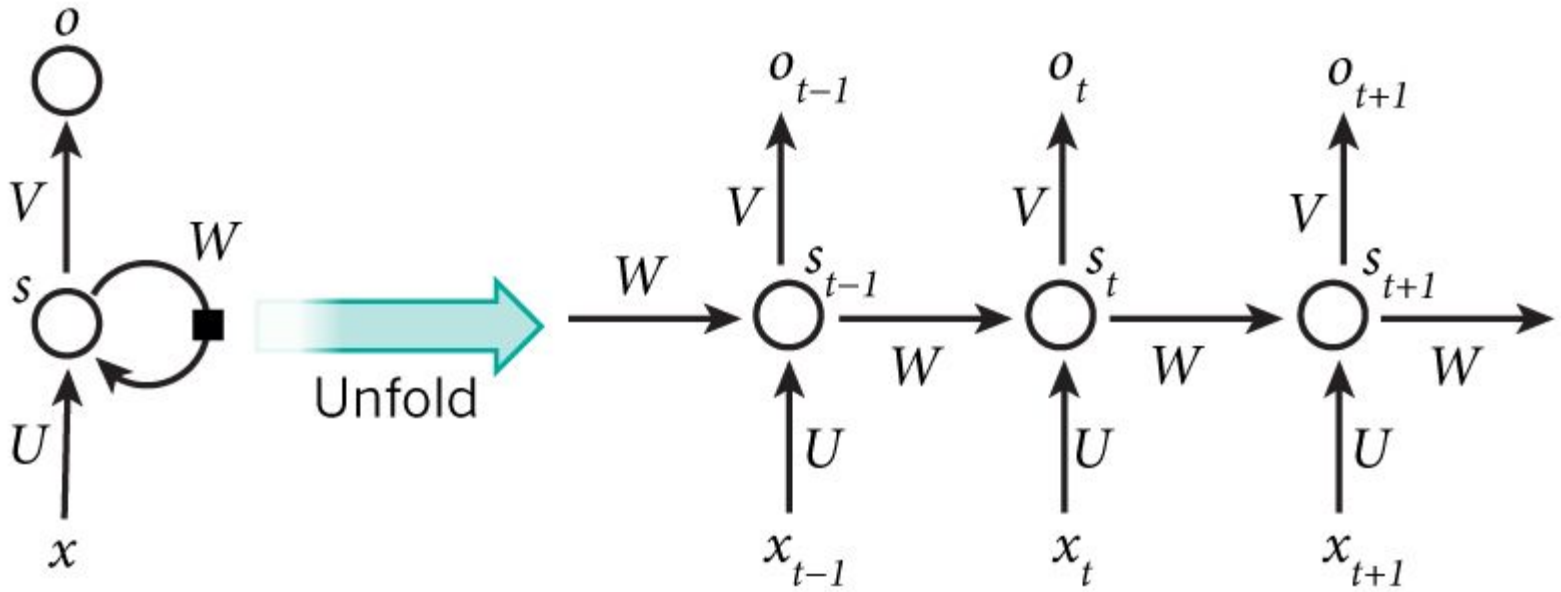
- Generate output, *y*, at each time step or at the end of the time series
  - Can be generated deterministically or sampled
  - May or may not be the same type as the input
  - Can model a single prediction of the next input or a joint prediction of the next *n* inputs

$$y_k = q_\theta(h_k) \text{ or } y_k \sim q_\theta(y_k|h_k)$$

Recurrent Neural Networks - General Idea

- Optimized via backprop through time
  - Equivalent to backprop and reverse-mode auto-differentiation
  - Costly to compute gradients for higher time steps
  - Number of application of chain rule proportional to depth of data
  - Need to store the gradient for each timestep

Simple Recurrent Neural Networks Diagram



http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/

Choices for Likelihood Functions

- For discrete output:
  - Use softmax to generate multinomial distribution from RNN output
- For continuous output:
  - Use RNN output as parameters for a chosen probability density function

Pros and Cons of Vanilla RNN

Cons:

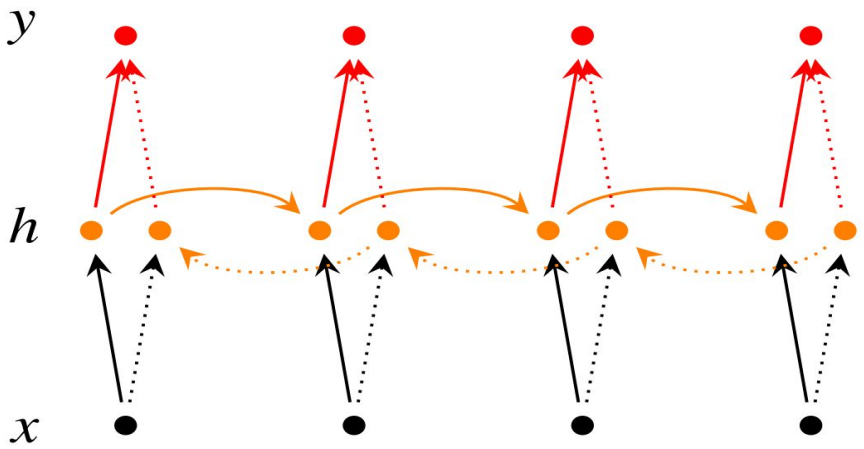
- We cannot answer any query about the joint distribution
  - Only makes forward inference, no backwards looking inference or interpolation
- The gradient explodes/decays exponentially with time making training using first order optimization methods challenging
- Storing gradients for all time steps is memory intensive

Pros:

- Uses likelihood functions
- Can handle any length of input sequences
- Trainable on large amounts of data without needing to establish priors or structure

Bidirectional RNN

Problem: For classification you want to incorporate information from words both preceding and following



$$\vec{h}_t = f(\vec{W}x_t + \vec{V}\vec{h}_{t-1} + \vec{b})$$

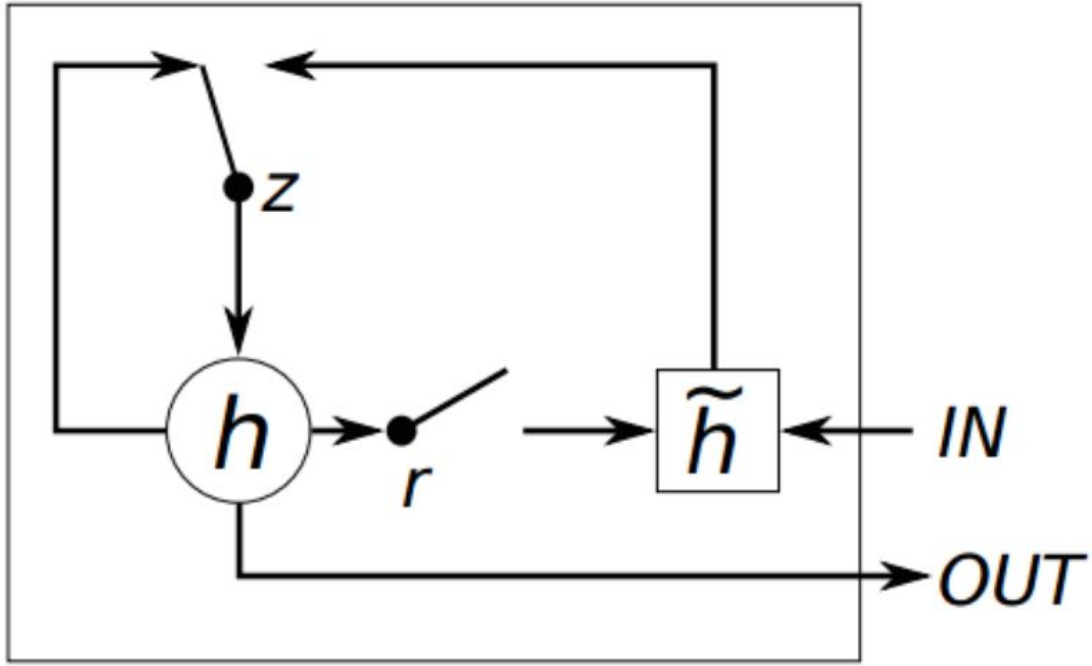
$$\overleftarrow{h}_t = f(\overleftarrow{W}x_t + \overleftarrow{V}\overleftarrow{h}_{t+1} + \overleftarrow{b})$$

$$y_t = g(U[\vec{h}_t; \overleftarrow{h}_t] + c)$$

$h = [\vec{h}; \overleftarrow{h}]$ now represents (summarizes) the past and future around a single token.

http://cs224d.stanford.edu/lectures/CS224d-Lecture8.pdf

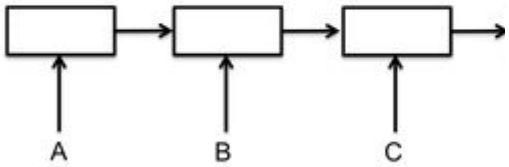
Gated Recurrent Unit



https://cs224d.stanford.edu/reports/BergerMark.pdf

Encoder RNNs

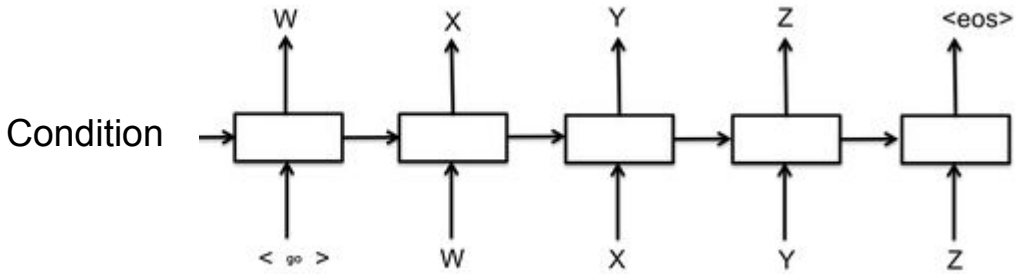
Convert sequential data into a compressed representation



https://www.tensorflow.org/versions/r0.10/tutorials/seq2seq/index.html

Decoder RNNs

Predict sequential data given an initial condition (inference)



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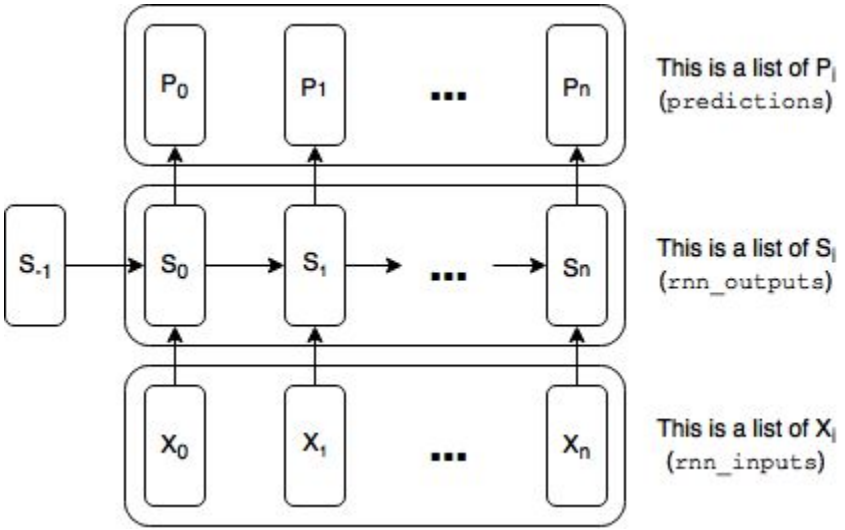
Application of RNNs

Recall what an RNN looks like:



http://r2rt.com/recurrent-neural-networks-in-tensorflow-ii.html

Application of RNNs

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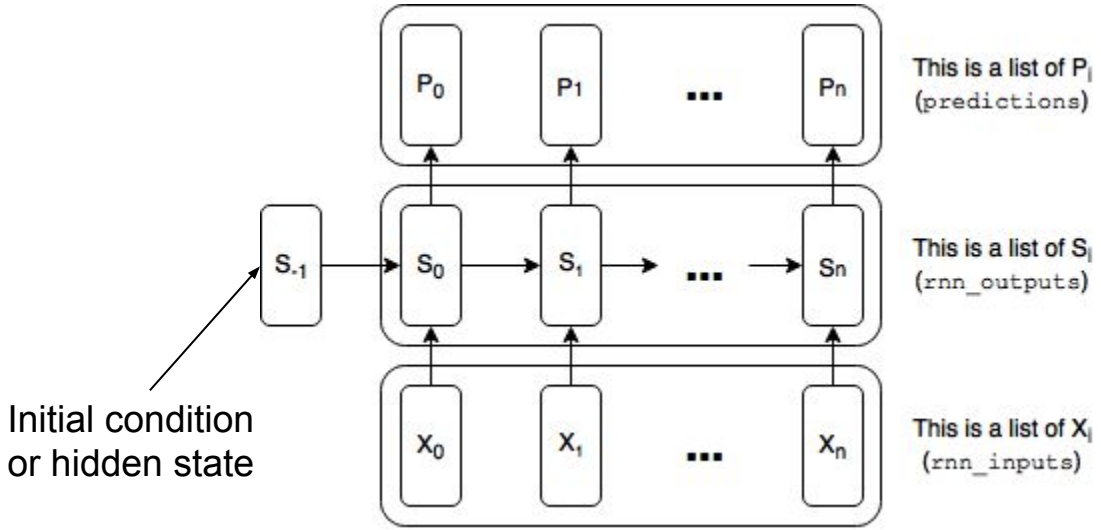

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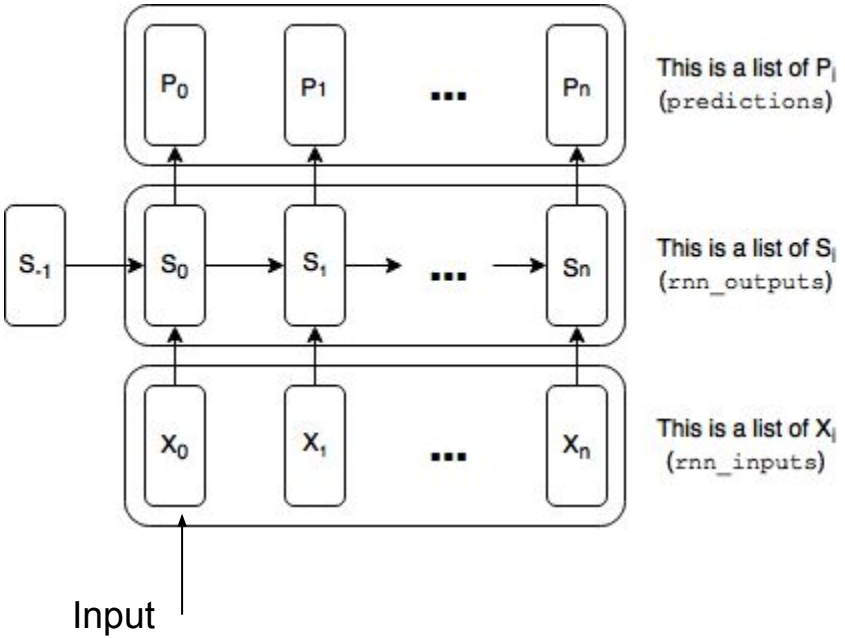

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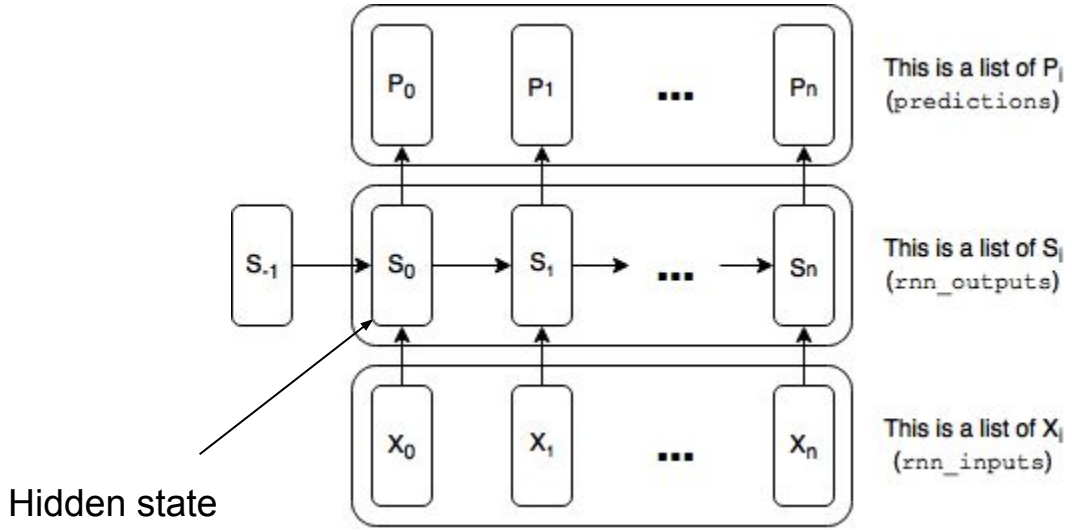

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Application of RNNs

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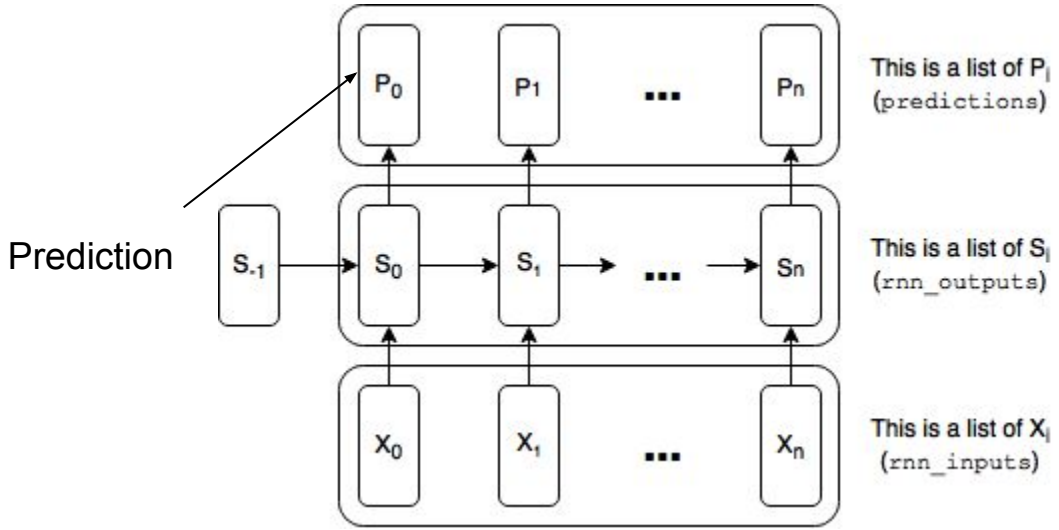
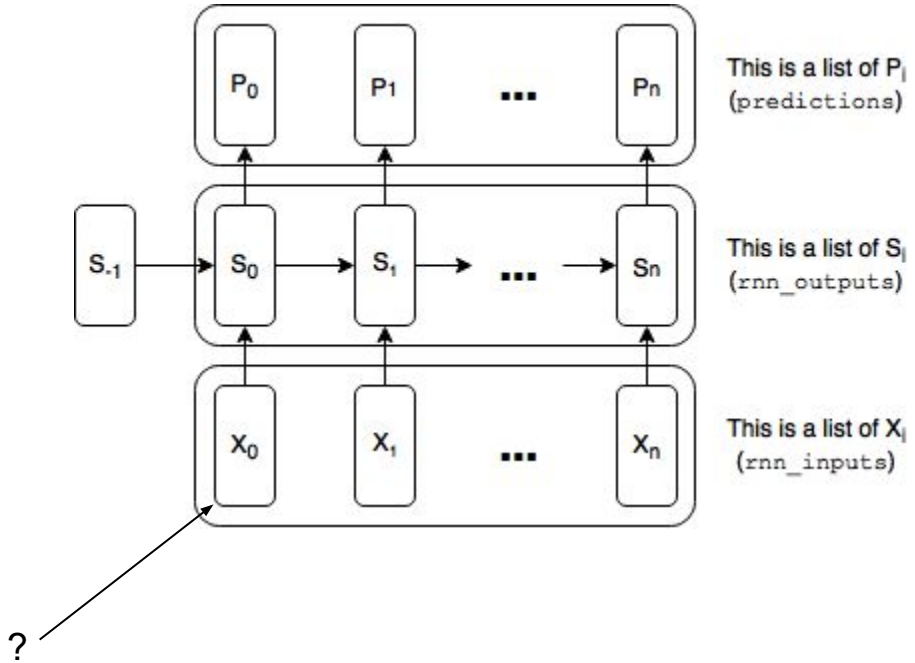


http://r2rt.com/recurrent-neural-networks-in-tensorflow-ii.html

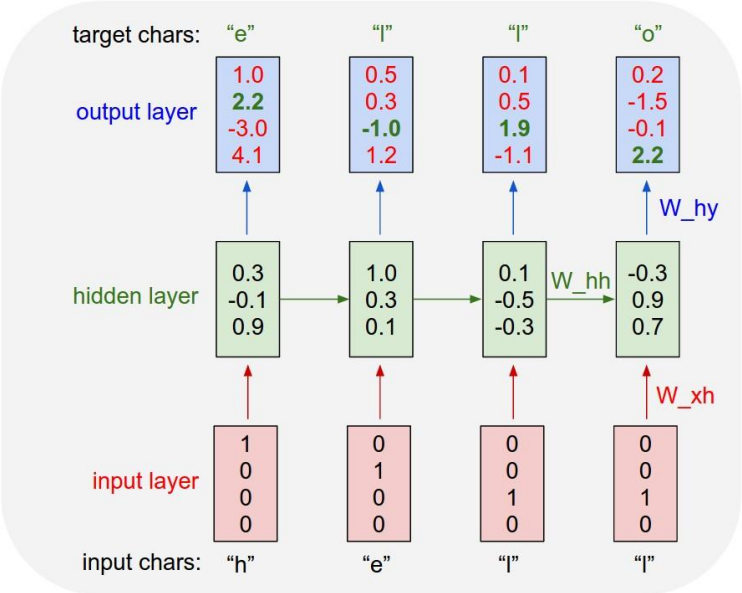
What should our inputs be?



http://r2rt.com/recurrent-neural-networks-in-tensorflow-ii.html

Application: Character-level language model

Predict next character given a string of characters



http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Text generation

Trained on a concatenation of essays written by some startup guru using a 2-layer LSTM with 512 hidden nodes. Better than Markov Models.

```
The surprised in investors weren’t going to raise money. I’m not the
company with the time there are all interesting quickly, don’t have to get
off the same programmers. There’s a super-angel round fundraising, why do
you can do. If you have a different physical investment are become in
people who reduced in a startup with the way to argument the acquirer could
see them just that you’re also the founders will part of users’ affords
that and an alternation to the idea. [2] Don’t work at first member to see
the way kids will seem in advance of a bad successful startup. And if you
have to act the big company too.
```

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Text generation

Locally the text looks correct, but upon closer inspection we find mistakes in the grammar and no coherent discourse (longer range correlations).

The surprised in investors weren't going to raise money. I'm**not the company with the time** there are all interesting quickly, don't have to get off the same programmers. There's a super-angel**round fundraising**, **why do you can do**. If you have a different **physical investment are become** in **people who reduced in a startup** with the way to argument the acquirer could see them just that **you're also the founders will part** of users' affords that and an **alternation to the idea**. [2] **Don't work at first member** to see the way kids will seem in advance of a bad successful startup. And if you have to act the big company too.

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Text generation: Shakespeare plays

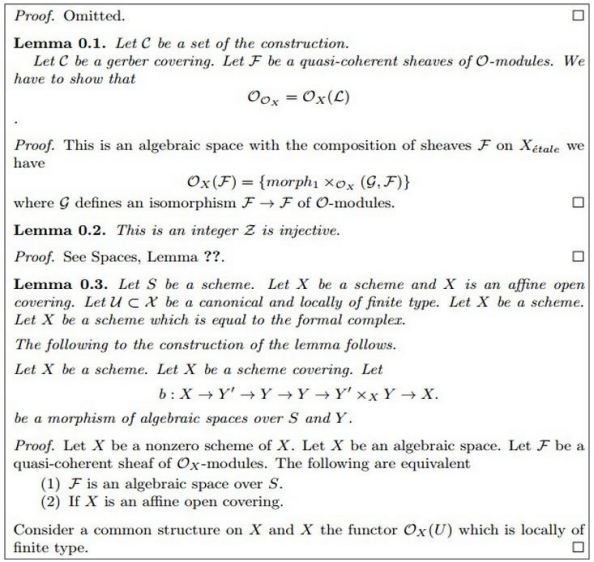
The model correctly simulates the play structure (and almost generates interesting stories)

```
DUKE VINCENTIO:
Well, your wit is in the care of side and that.

Second Lord:
They would be ruled after this chamber, and
my fair nues begun out of the fact, to be conveyed,
Whose noble souls I'll have the heart of the wars.

Clown:
Come, sir, I will make did behold your worship.

VIOLA:
I'll drink it.
```

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Text generation: Better than you at LaTeX

Dataset is Algebraic Geometry LaTeX source files. Sampled code almost compiles, sometimes chooses to omit proofs (as one does). Note that some long environments did not close, as some recurrent features are not generated.



Proof. Omitted. □

Lemma 0.1. *Let $\mathcal{C}$ be a set of the construction.*

Let $\mathcal{C}$ be a gerber covering. Let $\mathcal{F}$ be a quasi-coherent sheaves of $\mathcal{O}$-modules. We have to show that

$$\mathcal{O}_{\mathcal{O}_X} = \mathcal{O}_X(\mathcal{L})$$

.

Proof. This is an algebraic space with the composition of sheaves $\mathcal{F}$ on $X_{\acute{e}tale}$ we have

$$\mathcal{O}_X(\mathcal{F}) = \{morph_1 \times_{\mathcal{O}_X} (\mathcal{G}, \mathcal{F})\}$$

where $\mathcal{G}$ defines an isomorphism $\mathcal{F} \to \mathcal{F}$ of $\mathcal{O}$-modules. □

Lemma 0.2. *This is an integer $\mathcal{Z}$ is injective.*

Proof. See Spaces, Lemma ??. □

Lemma 0.3. *Let S be a scheme. Let X be a scheme and X is an affine open covering. Let $\mathcal{U} \subset \mathcal{X}$ be a canonical and locally of finite type. Let X be a scheme. Let X be a scheme which is equal to the formal complex.*

The following to the construction of the lemma follows.

Let X be a scheme. Let X be a scheme covering. Let

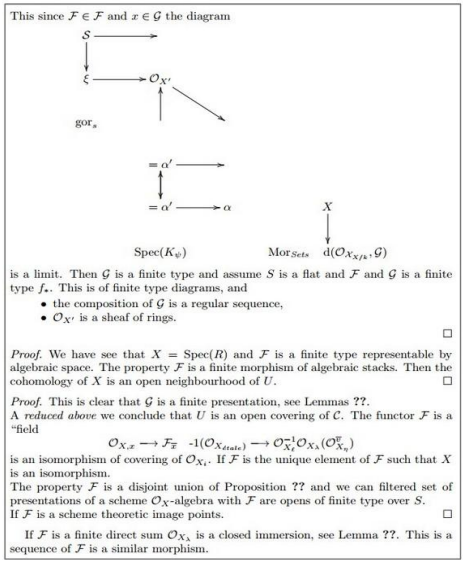
$$b : X \to Y' \to Y \to Y \to Y' \times_X Y \to X.$$

be a morphism of algebraic spaces over S and Y.

Proof. Let X be a nonzero scheme of X. Let X be an algebraic space. Let $\mathcal{F}$ be a quasi-coherent sheaf of $\mathcal{O}_X$-modules. The following are equivalent

(1) $\mathcal{F}$ is an algebraic space over S.
(2) If X is an affine open covering.

Consider a common structure on X and X the functor $\mathcal{O}_X(U)$ which is locally of finite type. □



This since $\mathcal{F} \in \mathcal{F}$ and $x \in \mathcal{G}$ the diagram

$$\begin{array}{ccc} S & \longrightarrow & \\ \downarrow & & \\ \xi & \longrightarrow & \mathcal{O}_{X'} \\ & \nearrow & \\ \mathrm{gor}_s & & \end{array}$$

$$\begin{array}{ccc} & = \alpha' & \longrightarrow \\ & \updownarrow & \\ = \alpha' & \longrightarrow & \alpha \end{array} \qquad \begin{array}{c} X \\ \downarrow \end{array}$$

$$\mathrm{Spec}(K_\psi) \qquad \mathrm{Mor}_{Sets} \quad \mathrm{d}(\mathcal{O}_{X_{\acute{e}t}}, \mathcal{G})$$

is a limit. Then $\mathcal{G}$ is a finite type and assume S is a flat and $\mathcal{F}$ and $\mathcal{G}$ is a finite type f_*. This is of finite type diagrams, and

- the composition of $\mathcal{G}$ is a regular sequence,
- $\mathcal{O}_{X'}$ is a sheaf of rings.

□

Proof. We have see that $X = \mathrm{Spec}(R)$ and $\mathcal{F}$ is a finite type representable by algebraic space. The property $\mathcal{F}$ is a finite morphism of algebraic stacks. Then the cohomology of X is an open neighbourhood of U. □

Proof. This is clear that $\mathcal{G}$ is a finite presentation, see Lemmas ??.
A *reduced above* we conclude that U is an open covering of $\mathcal{C}$. The functor $\mathcal{F}$ is a "field

$$\mathcal{O}_{X,x} \longrightarrow \mathcal{F}_{\overline{x}} \quad \text{-1}(\mathcal{O}_{X_{\acute{e}tale}}) \longrightarrow \mathcal{O}_{X_t}^{-1}\mathcal{O}_{X_\lambda}(\mathcal{O}_{X_\eta}^{\mathbb{E}})$$

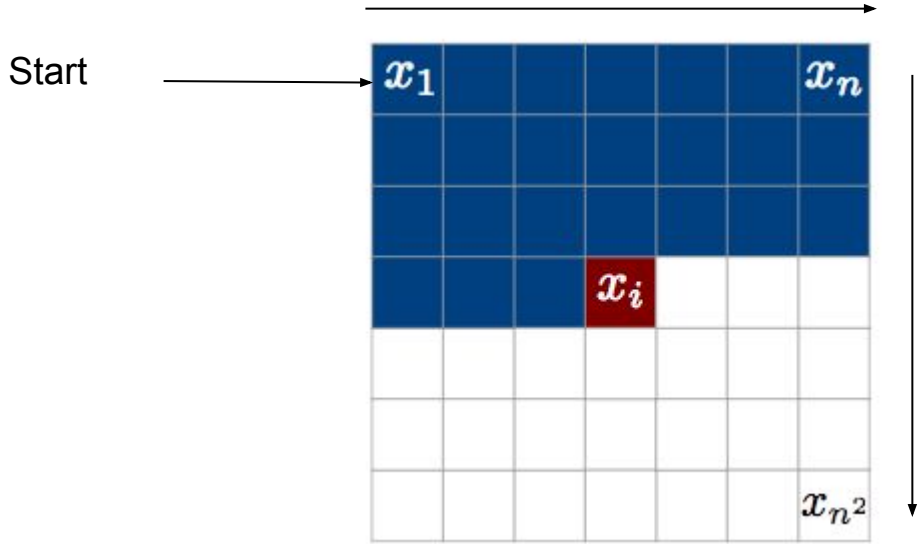
is an isomorphism of covering of $\mathcal{O}_{X_i}$. If $\mathcal{F}$ is the unique element of $\mathcal{F}$ such that X is an isomorphism.
The property $\mathcal{F}$ is a disjoint union of Proposition ?? and we can filtered set of presentations of a scheme $\mathcal{O}_X$-algebra with $\mathcal{F}$ are opens of finite type over S.
If $\mathcal{F}$ is a scheme theoretic image points. □

If $\mathcal{F}$ is a finite direct sum $\mathcal{O}_{X_\lambda}$ is a closed immersion, see Lemma ??. This is a sequence of $\mathcal{F}$ is a similar morphism.

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Pixel-RNN (van den Oord et al. 2016)

Generative model of images



https://arxiv.org/pdf/1601.06759v3.pdf

Pixel-RNN (van den Oord et al. 2016)

Generative model of images

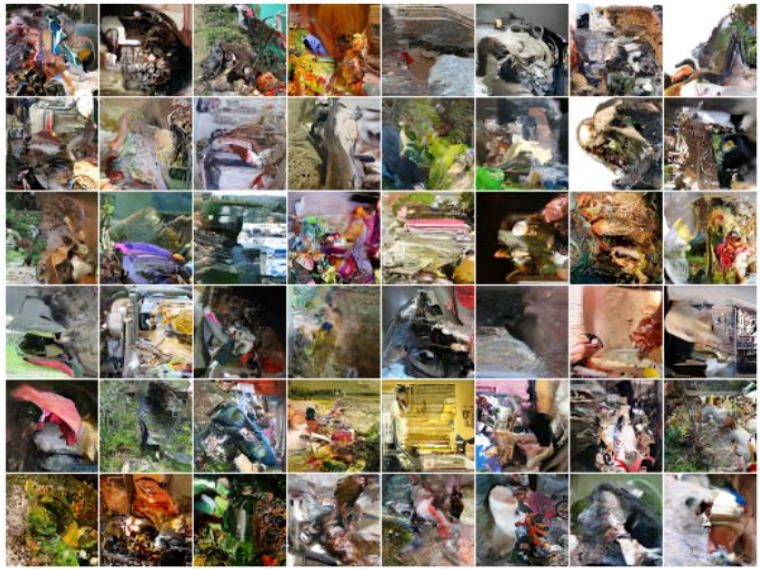
Note: completions can only go one way

Figure 1. Image completions sampled from a PixelRNN.

https://arxiv.org/pdf/1601.06759v3.pdf

Pixel-RNN (van den Oord et al. 2016)

Generative model of images



https://arxiv.org/pdf/1601.06759v3.pdf

Teacher forcing (Doya 1993)

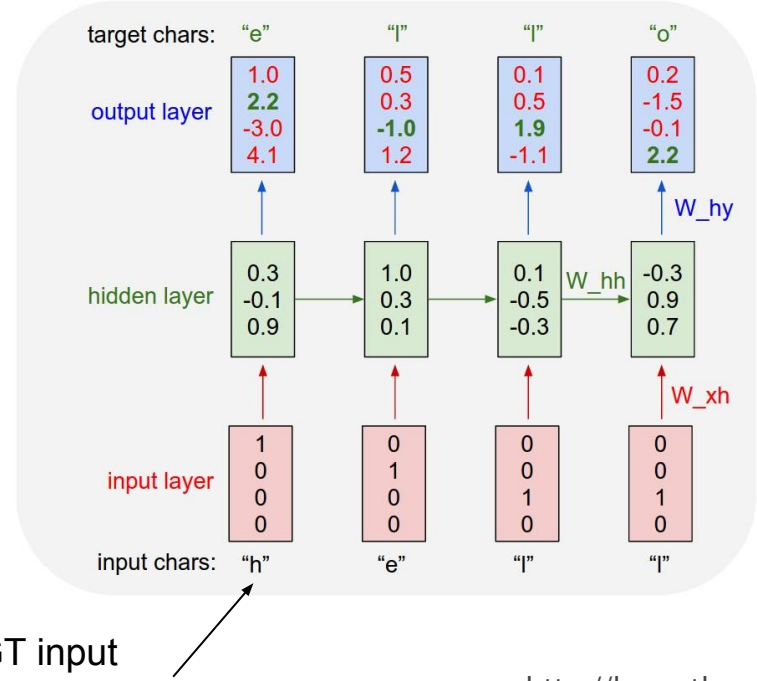
This is what an RNN output looks like at the beginning (compounding errors)

```
tyntd-iafhatawiaoihrdemot  lytdws  e ,tfti, astai f ogoh eoase rrranbyne 'nhthnee e
plia tklrgd t o idoe ns,smtt   h ne etie h,hregtrs nigtike,aoaenns lng
```

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Teacher forcing (Doya 1993)

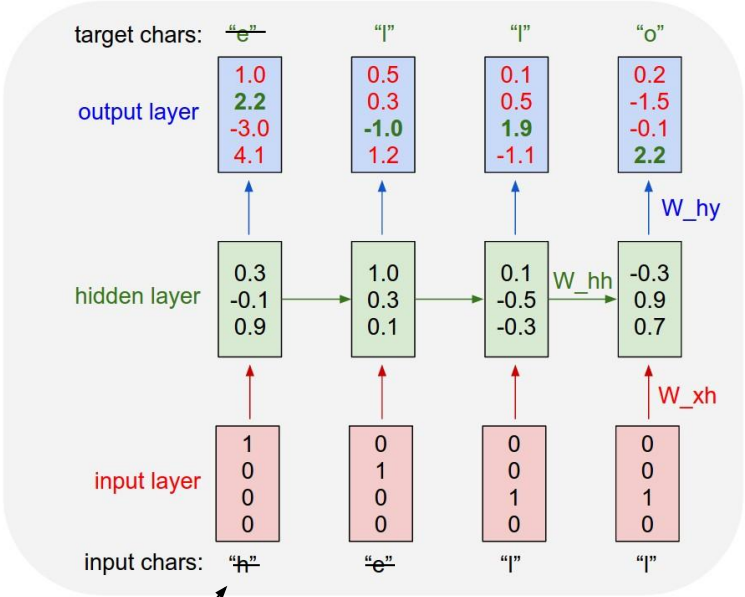
Use ground truth inputs during training to make training more stable and prevent exploding gradients.



http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Teacher forcing (Doya 1993)

At inference a sample from your posterior distribution is used.



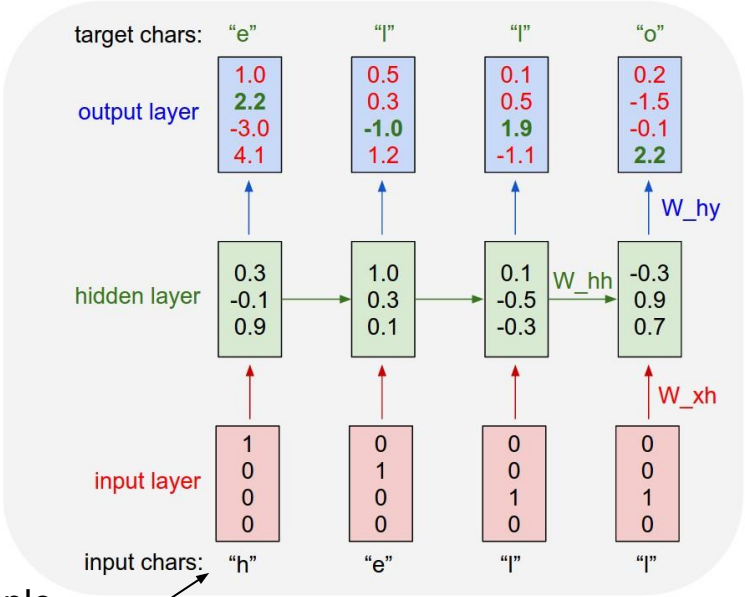
Previous samples

Mismatch between training and inference!

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Scheduled sampling (S. Bengio et al., 2015)

Use an schedule during training to progressively move from using GT inputs to using samples.



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Initial condition

What can we use as an initial condition?

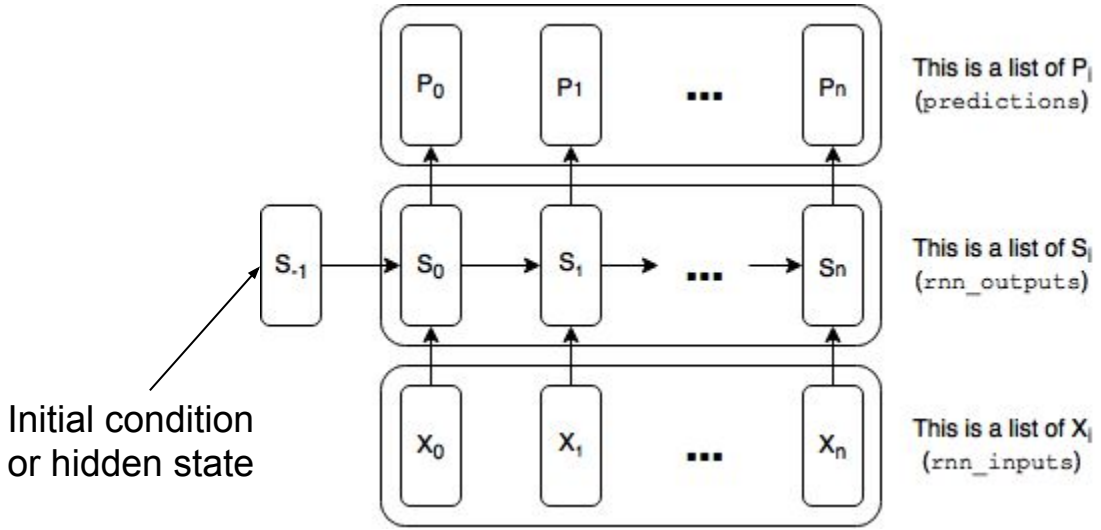

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Image captioning (Kiros et al. Vinyals et al.., …)

Predict caption given an image

Obtain a vector representation of an image (e.g. using a CNN)

https://research.googleblog.com/2016/09/show-and-tell-image-captioning-open.html

Image captioning (Kiros et al. Vinyals et al.., …)

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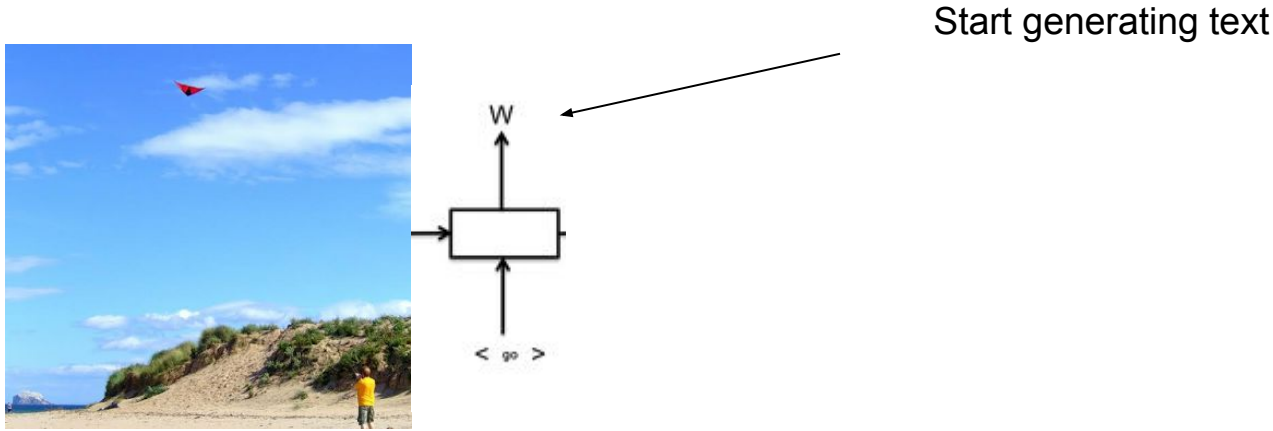

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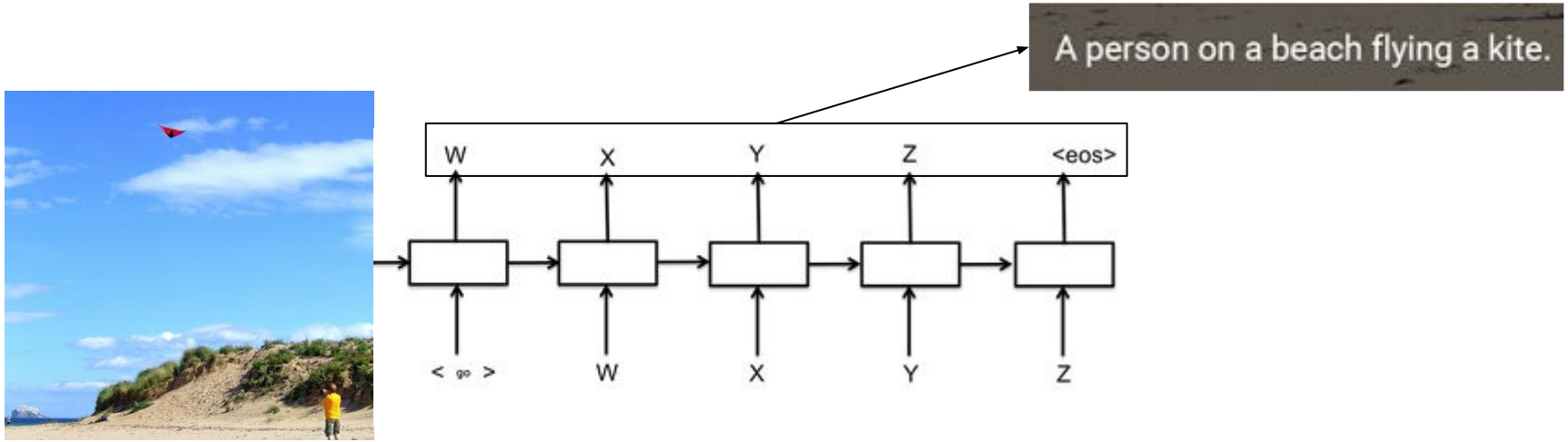

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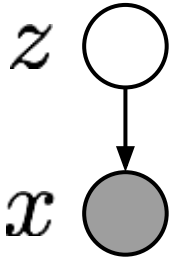
Code example

Invertible Models

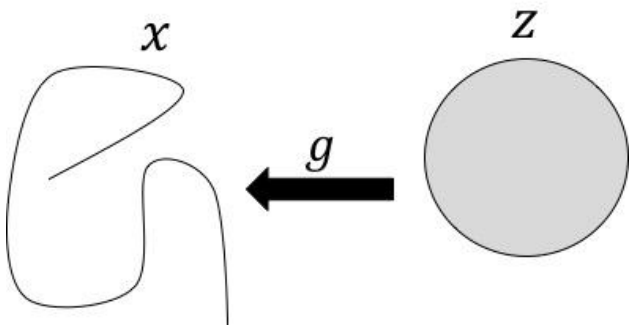
Invertible Models



- Class of probabilistic generative models with:
  - Exact sampling $x \sim p(x)$
  - Exact inference $p(z|x) = p(z)p(x|z)/p(x)$
  - Exact likelihood computation $p(x) = \int p(x|z)\, p(z)\, dz$
- Relies on exploiting the change-of-variable formula for bijective functions

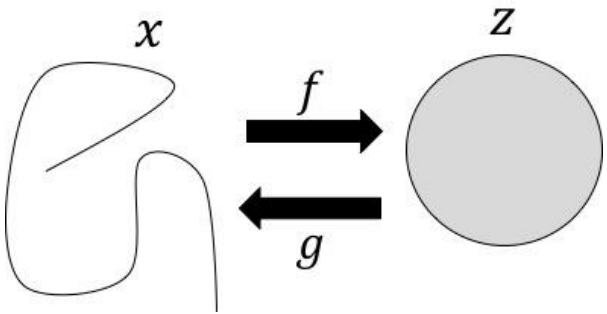
Generative Procedure

- Start with a latent space that is easy to sample from
  - e.g. $z \sim p_Z(z) = \mathcal{N}(0, I)$
- Pass the sampled point through a *generator function*
  - $x = g(z)$
- This gives us <u>exact sampling</u> ✓
- Similar procedure as for VAEs except the generator function is deterministic



Inference

- Choose *g* such that the mapping is *bijective*
  - Each point x has exactly one associated point in latent space, and vice versa
  - Therefore *g* has an inverse function $f = g^{-1}$
- Given an arbitrary *x*, directly compute $z = f(x)$



Exact inference ✓

Likelihood Computation

- Given a random variable *Z* and a bijection *X = g(Z)* ⇔ *Z = f(X)*, the pdf of *X* can be expressed in terms of the pdf of *Z*:

$$p_X(x) = p_Z\big(f(x)\big)\left|\det\left(\frac{\partial f(x)}{\partial x^T}\right)\right|$$

Jacobian matrix

- Due to the bijection constraint, there is only one possible *z* for a given *x*. Hence the likelihood function is reduced to the above pdf for *X = g(Z)*.
  - Exact likelihood computation ✓

Recall: Change of Variables for 2D

$$Pr(z_1, z_2 \in R_z) = \iint_{R_z} p_z(z_1, z_2)\, dz_1\, dz_2$$

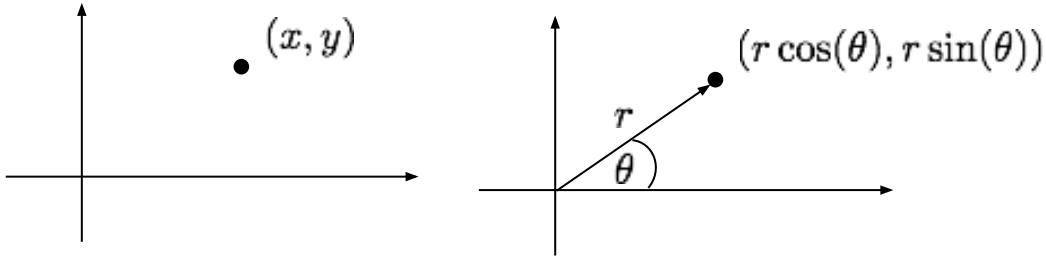
Let R_x be identical to R_z but specified in the $x_1 - x_2$ plane

$$\iint_{R_x} p_z(z_1(x_1, x_2), z_2(x_1, x_2)) \left| \frac{\partial(z_1, z_2)}{\partial(x_1, x_2)} \right| dx_1\, dx_2$$

$$Pr(z_1, z_2 \in R_z) = Pr(x_1, x_2 \in R_x) = \iint_{R_x} p_x(x_1, x_2)\, dx_1\, dx_2$$

$$p_x(x_1, x_2) = p_z(z_1(x_1, x_2), z_2(x_1, x_2)) \left| \frac{\partial(z_1, z_2)}{\partial(x_1, x_2)} \right|$$

Example: Cartesian to Polar Coordinates



Cartesian

$p_{XY}(x, y)$

Polar

$p_{r\theta}(r, \theta) = ?$

$$J = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -r\sin(\theta) \\ \sin(\theta) & r\cos(\theta) \end{pmatrix}$$

$$\Rightarrow |\det J| = |r\cos^2(\theta) + r\sin^2(\theta)| = |r|$$

$$p_{r\theta}(r, \theta) = p_{XY}(r\cos(\theta), r\sin(\theta))|\det J| = p_{XY}(r\cos(\theta), r\sin(\theta))\, r$$

Invertible Approach: Challenges

- Invertible approach gives us exact sampling, inference and likelihood computation.
- There are still three big questions to answer:
  a. How to parameterize expressive bijective functions?
  b. How to efficiently compute a large Jacobian matrix?
  c. How to efficiently compute the determinant of a large matrix?

Parameterization of Bijective Functions

- Dinh et al. 2016 propose to use *affine coupling layers*:

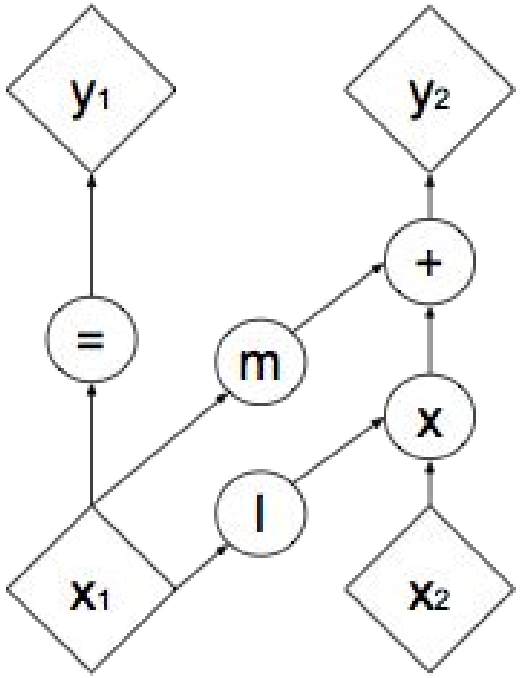
$$y_{1:d} = x_{1:d}$$

$$y_{d+1:D} = x_{d+1:D} \odot \exp\left(l(x_{1:d})\right) + m(x_{1:d})$$

- Flexibility can be gained by increasing the complexity of l and m.

$$x_{1:d} = y_{1:d}$$

$$x_{d+1:D} = \left(y_{d+1:D} - m(y_{1:d})\right) \odot \exp\left(-l(y_{1:d})\right)$$



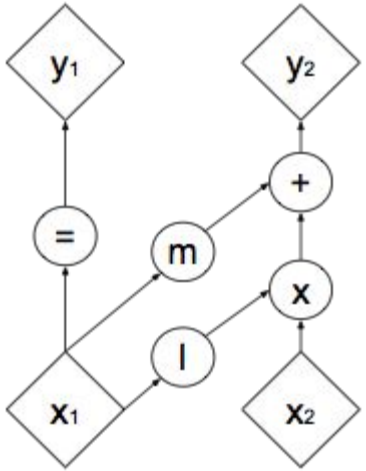
L. Dinh, J. Sohl-Dickstein, and S. Bengio, “Density estimation using Real NVP,” arXiv.org, vol. cs.LG. 27-May-2016.

Jacobian Computation

- The Jacobian of the transformation

$$y_{1:d} = x_{1:d}$$

$$y_{d+1:D} = x_{d+1:D} \odot \exp\left(l(x_{1:d})\right) + m(x_{1:d})$$



can be expressed as:

$$\frac{\partial y}{\partial x^T} = \begin{bmatrix} \mathbb{I}_d & 0 \\ \frac{\partial y_{d+1:D}}{\partial x_{1:d}^T} & \operatorname{diag}\left(\exp(l)\right) \end{bmatrix} \begin{matrix} y_{1:d} \\ y_{d+1:D} \end{matrix} \qquad \frac{\partial y_i}{\partial x_j}$$

$$x_{1:d} \qquad x_{d+1:D}$$

Determinant Computation

- For a 2 x 2 matrix

$$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - bc$$

- For a triangular matrix

$$\det \begin{pmatrix} a & 0 & 0 & 0 \\ b & c & 0 & 0 \\ d & e & f & 0 \\ w & x & y & z \end{pmatrix} = acfz$$

Determinant Computation

- The Jacobian in our example is a triangular matrix:

$$\frac{\partial y}{\partial x^T} = \begin{bmatrix} \mathbb{I}_d & 0 \\ \frac{\partial y_{d+1:D}}{\partial x_{1:d}^T} & \operatorname{diag}\big(\exp(l)\big) \end{bmatrix}$$

- Hence, its determinant is

$$\det \frac{\partial y}{\partial x^T} = \exp\left(\sum_j l(x_{1:d})_j\right)$$

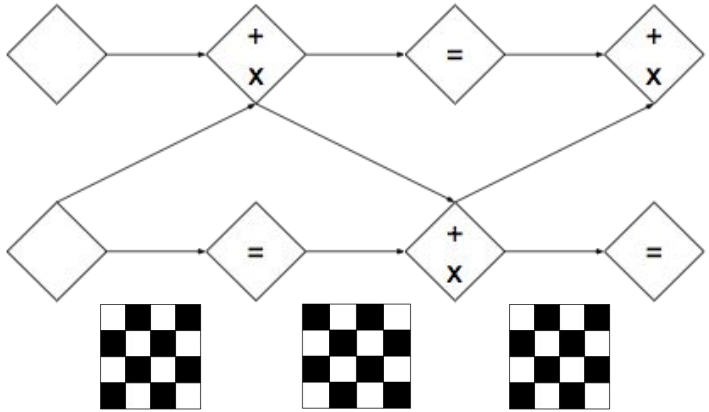
- Regardless of the lower-left block!

Masked Convolution

- For images choose *l* and *m* to be deep convnets
- Rather than explicitly partitioning the input, use binary mask instead:

$$y = b \odot x + (1 - b) \odot \left(x \odot \exp\left(l(b \odot x)\right) + m(b \odot x) \right)$$

- Masks applied in alternating checkerboard pattern

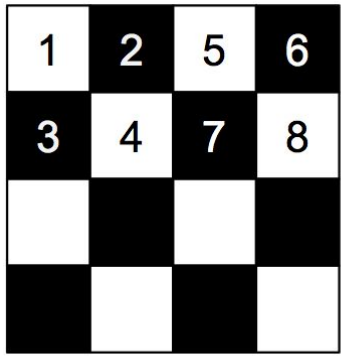


Dinh et al. 2016

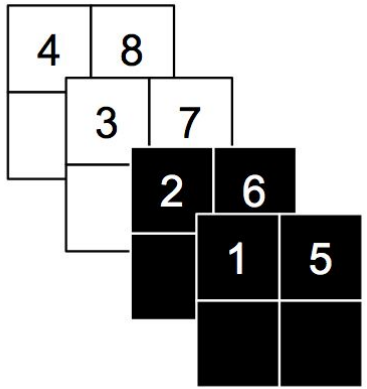
Multi-scale Architecture

- Squeezing operation reduces spatial resolution and increases channels

- At each scale use the following recipe:
  - Three coupling layers with alternating checkerboards
  - Squeezing operation
  - Three coupling layers with channel-wise masking



$$s \times s \times c$$



$$\frac{s}{2} \times \frac{s}{2} \times 4c$$

Checkerboard and channel-wise masks are <u>not redundant</u>

Dinh et al. 2016

Factoring out latent variables

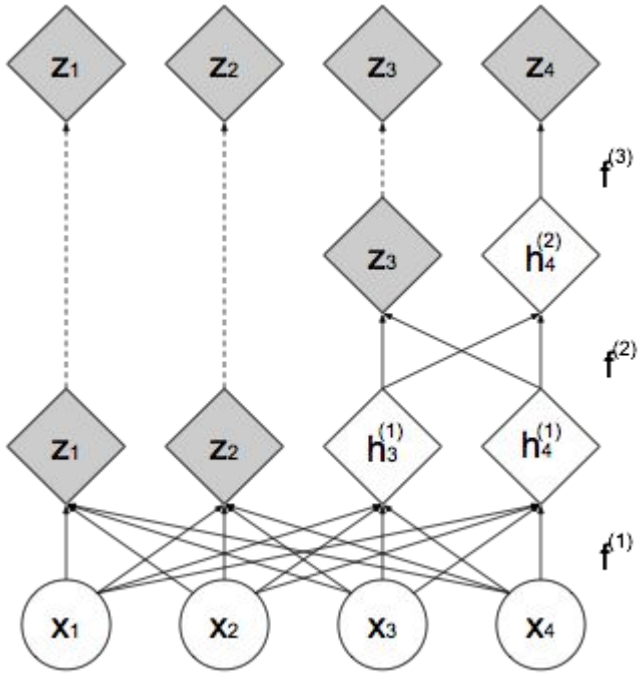
- Propagating full D-dimensional vector through all layers is expensive in computation and memory.
- Factor out half of the latent variables at regular intervals.

$$h^{(0)} = x$$

$$(z^{(i+1)}, h^{(i+1)}) = f^{(i+1)}(h^{(i)})$$

$$z^{(L)} = f^{(L)}(h^{(L-1)})$$

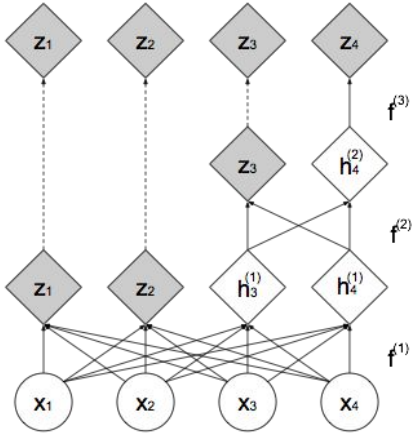
$$z = (z^{(1)}, \ldots, z^{(L)})$$



Dinh et al. 2016

Factoring out latent variables

- Variables factored out in lower layers capture noise and low-level details.
- Those in higher layers capture more abstract concepts



Dinh et al. 2016

more latent dimensions → fewer latent dimensions

Samples

LSUN Tower Category

x10

Dinh et al. 2016

Latent Manifold

Dinh et al. 2016

Compression Results

	CIFAR-10	Imagenet (32 x 32)	Imagenet (64 x 64)
Pixel RNN	3.00	3.86	3.63
Real NVP	3.49	4.28	4.01
Conv DRAW	3.59	< 4.40	< 4.10

bits/dim on test set

Achieves competitive performance relative to:

- Pixel RNN (an autoregressive approach)
- Convolutional DRAW (a VAE approach)

Dinh et al. 2016

Related Work

- Real NVP (Dinh et al. 2016) was able to get good results on challenging datasets and is getting a lot of attention for it. But other previous works have also explored the role of bijective functions for density estimation.
  - Deep density models (Rippel & Adams 2013)
  - Non-linear Independent Components Estimation (Dinh et al. 2014)
  - Generalized Divisive Normalization (Ballé et al. 2015)

L. Dinh, J. Sohl-Dickstein, and S. Bengio, “Density estimation using Real NVP,” *arXiv.org*, vol. cs.LG. 27-May-2016.
O. Rippel and R. P. Adams, “High-Dimensional Probability Estimation with Deep Density Models,” *arXiv.org*, vol. stat.ML. 20-Feb-2013.
L. Dinh, D. Krueger, and Y. Bengio, “NICE: Non-linear Independent Components Estimation,” *arXiv.org*, vol. cs.LG. 30-Oct-2014.
J. Ballé, V. Laparra, and E. P. Simoncelli, “Density Modeling of Images using a Generalized Normalization Transformation,” *arXiv.org*, vol. cs.LG. 19-Nov-2015.

Recap + Comparison with Other Approaches

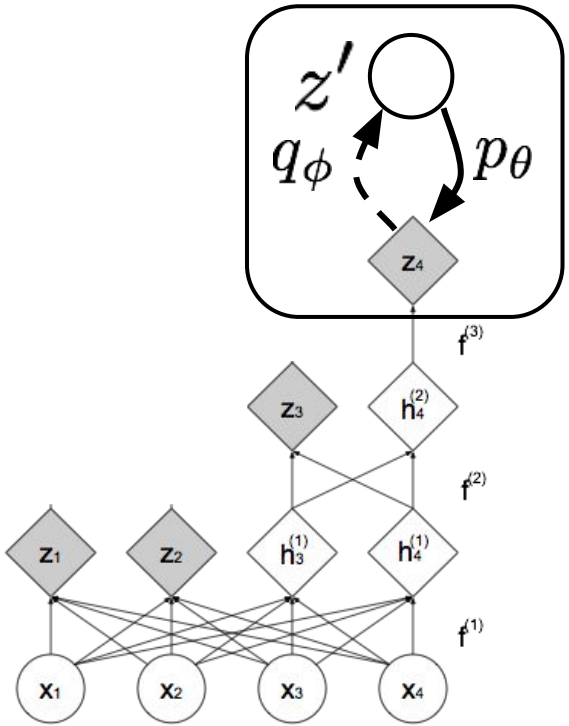
	VAE	Auto-regressive	GAN	Invertible Models
Exact Sampling	✓	✓	✓	✓
Exact Inference	✘	-	✘	✓
Exact Log-Likelihood	✘	✓	✘	✓

Invertible models have desirable characteristics but have two main drawbacks:

- Must use bijective functions with tractable Jacobian determinant
- Latent dimensionality is equal to the dimensionality of input

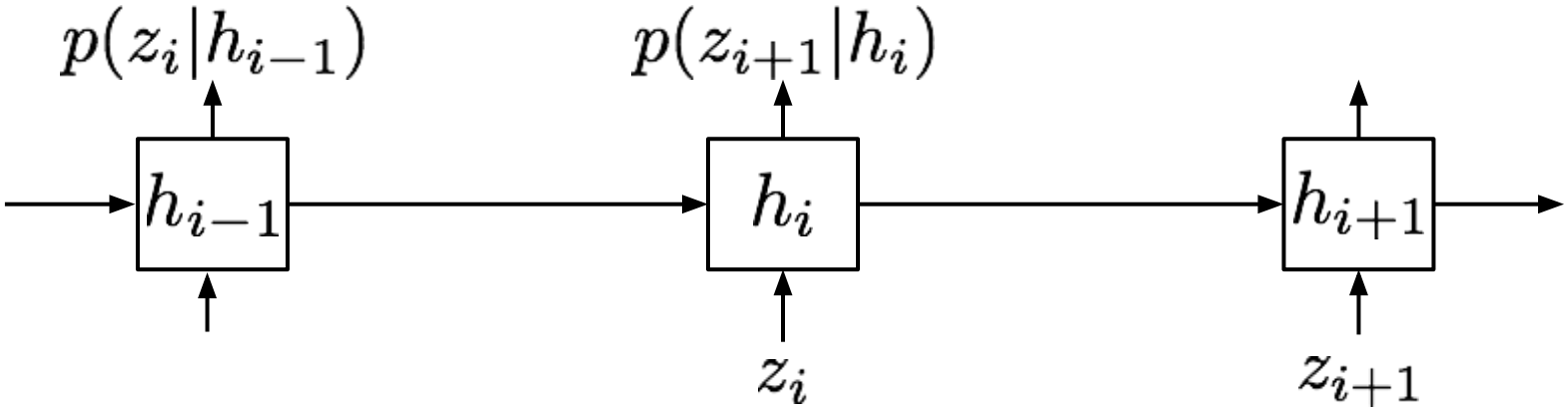
Invertible Models + VAEs

- Highest level latent variables are most important for the content of an image
- Instead of using a simple Gaussian prior, stack a VAE on top to get a more expressive distribution for these latent variables



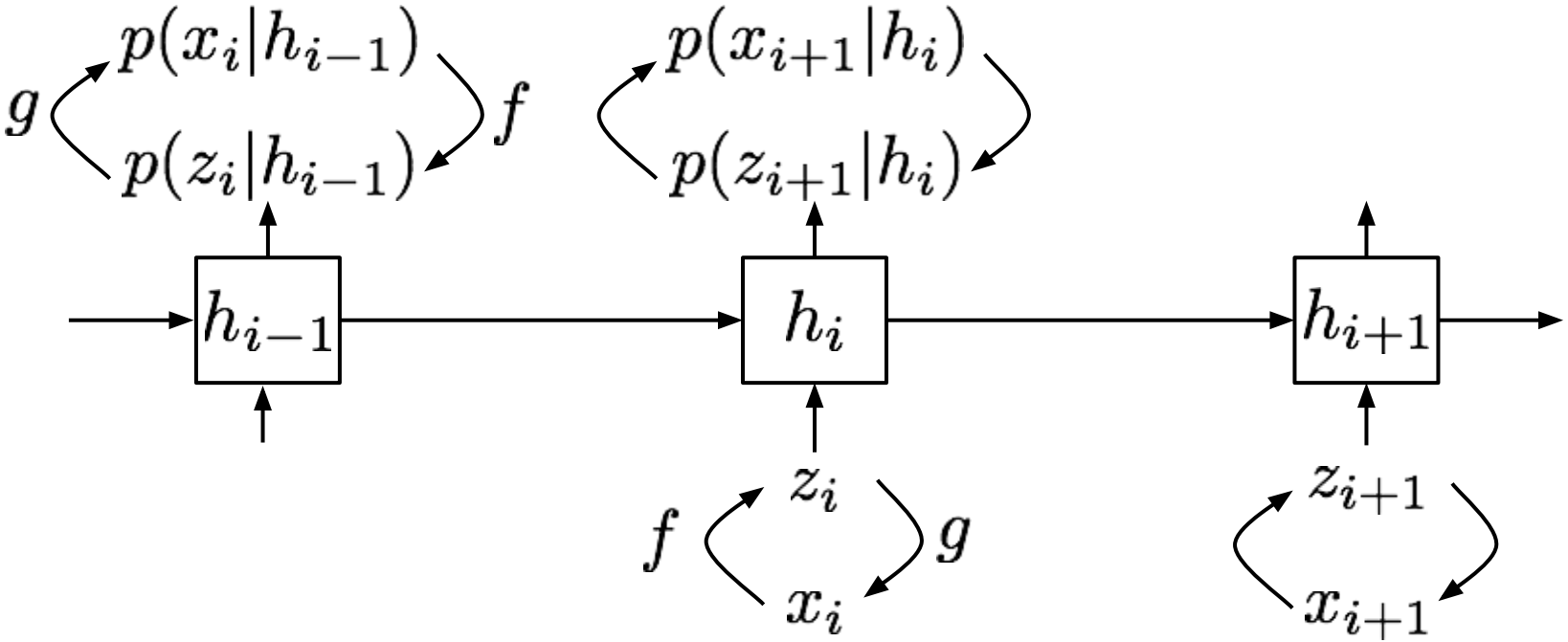
Invertible Models + Autoregressive

- Bijectivity gives another way to specify likelihood: dist. over z_i ⇔ dist. over x_i



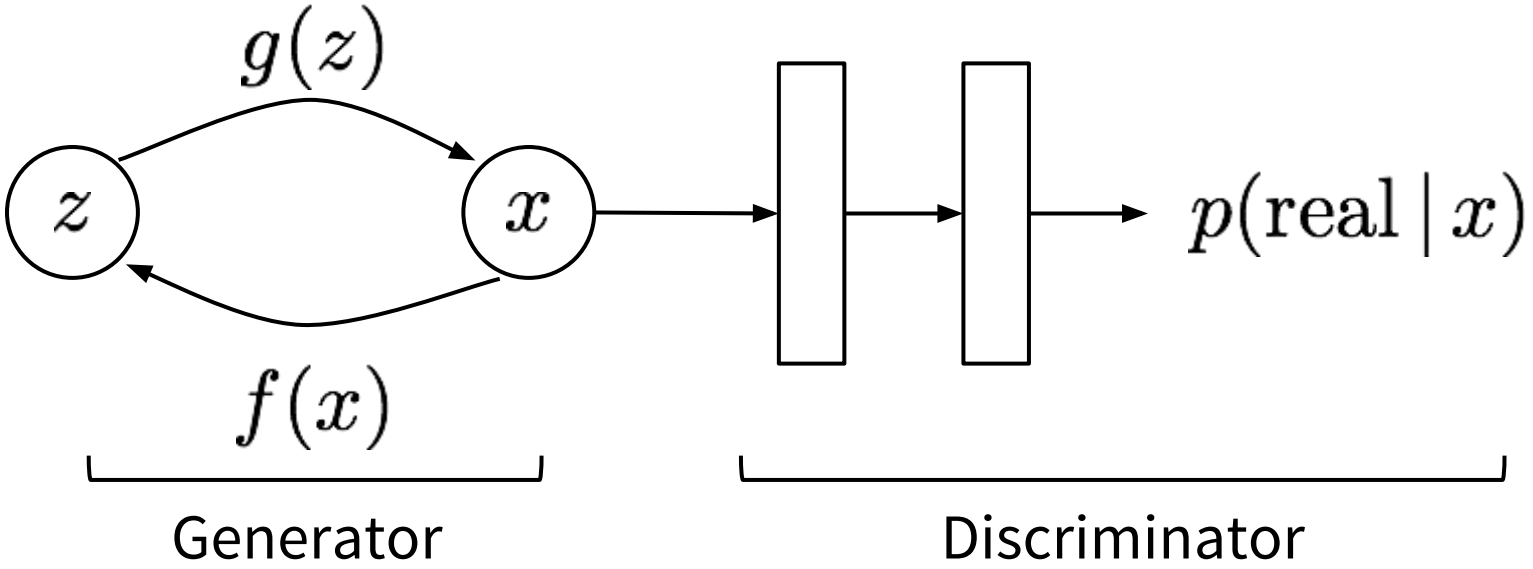
Invertible Models + Autoregressive

- Bijectivity gives another way to specify likelihood: dist. over z_i ⇔ dist. over x_i



Invertible Models + GANs

- Replacing a GAN's generator with a bijective function gives us inference for free:



- Existing work to invert the generator of a GAN (ALI of Dumoulin et al. 2016), (BiGAN of Donahue et al. 2016) but do not directly engineer the generator to be bijective.