A brief introduction to deep learning for generative modeling

Jakob Verbeek
INRIA, Grenoble, France

Breaking the Surface 2019
Biograd na Moru, Croatia

Plan for this presentation

1. Introduction to deep learning
    - Machine learning basics
    - Deep learning building blocks (MLP, convolution, back-propagation)
2. Deep generative models
    - Generative modeling basics
    - Generative adversarial networks
    - Variational autoencoders
    - Flow-based density estimation

Part I

Brief introduction to (deep) learning

Machine learning paradigms

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- **Unsupervised Learning**: discover patterns in unlabeled data
  - ex: cluster similar documents based on text content
- **Reinforcement Learning**: learning sequential decision making based on feedback or reward
  - ex: learning to play a game by winning or losing

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- Learning algorithms derive meaning out of data by using a **hierarchy of multiple layers** of units (*neurons*)
- Each layer computes linear function of its inputs, which is passed through a non linear function
- Learning = find optimal model parameters from data
    - ex: deep speech transcription system has 10-20M of parameters

A very brief history

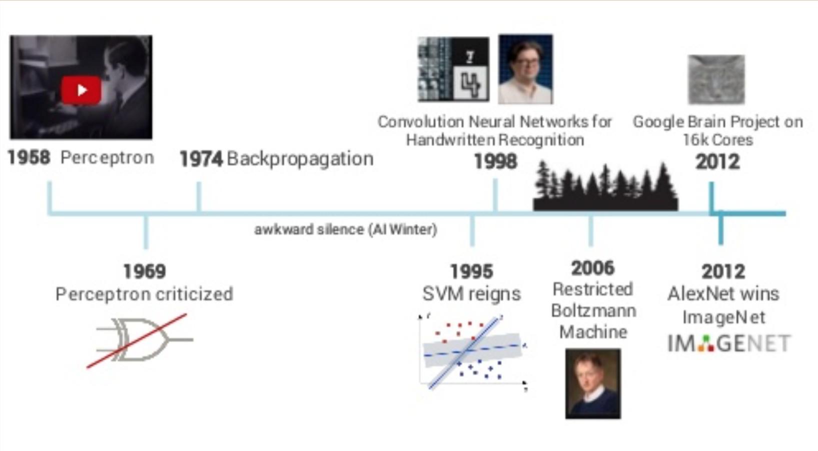

Figure from https://www.slideshare.net/LuMa921/deep-learning-a-visual-introduction

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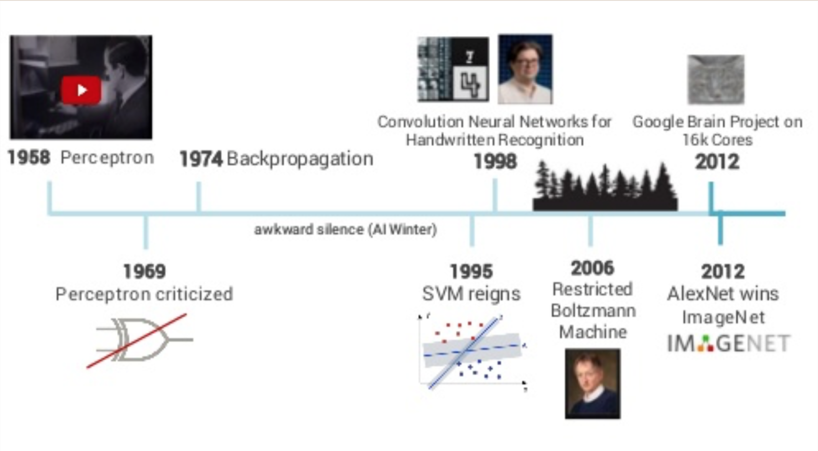

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- 2012 breakthrough due to
  - Lots of labeled data (ex: ImageNet)
  - Computation (ex: GPU)
  - Algorithmic & architectural progresses (ex: SGD, ReLU)

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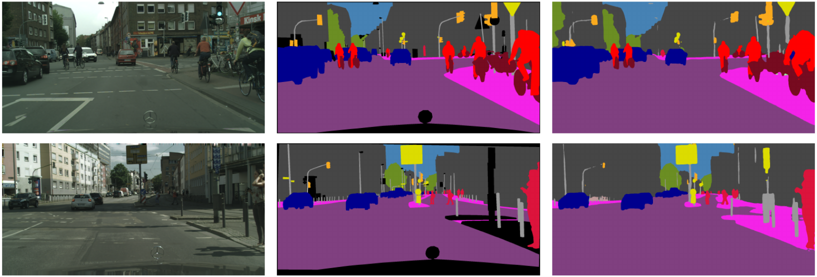

RGB Input Ground-truth Predictions

Semantic segmentation pixel labeling [Lin et al., 2017]

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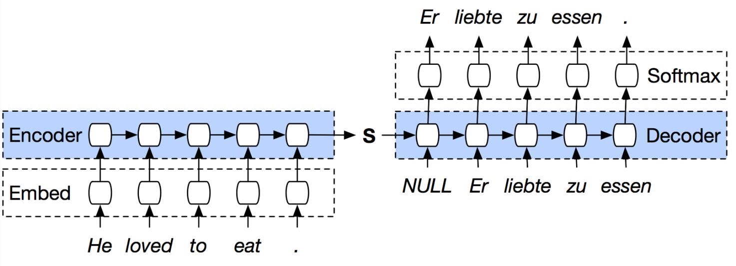

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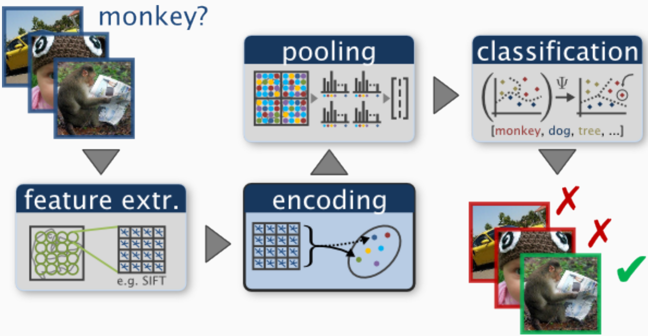

Image from [Chatfield et al., 2011]

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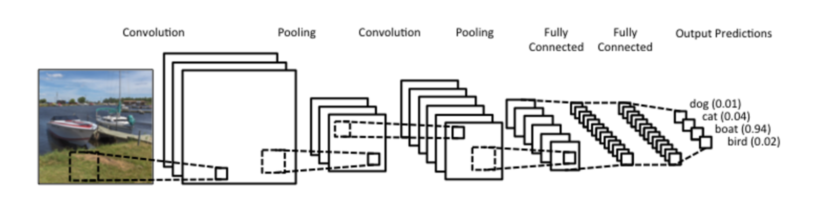

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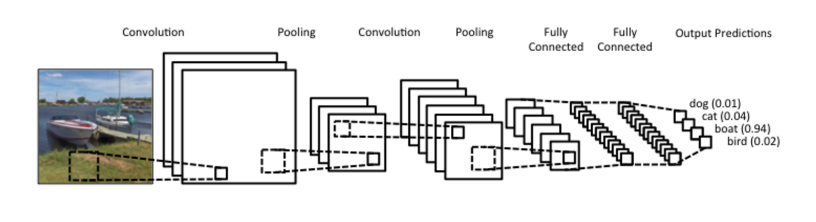

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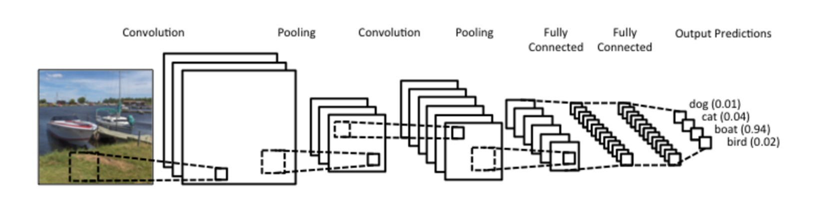
- Supervised learning from lots of labeled data



Training a model by empirical risk minimization

- Given labeled training data $(x_i, y_i)_{i=1...N}$ with $x_i \in \mathcal{X}, y_i \in \mathcal{Y}$
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  - $\{1, \ldots, K\}$: multi-class classification
  - $\mathbb{R}$: regression
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- Loss function L evaluates predictions, often convex

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- Not just risk minimization
  - Need to generalize to unseen examples
  - Occam's razor (favor simplicity)
  - Regularization: control the complexity of solutions

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- Linear regression example.
  - Assume linear relation between y and features $x \in \mathbb{R}^p$
  - $f(x) = w^T x + b$, parametrized by w, b in $\mathbb{R}^{p+1}$
  - L is often convex, $\Omega(f)$ often squared l_2-norm $||w||^2$.
  - Optimize by gradient descent: follow the steepest direction.
  - The problem is convex: local optimum is global.
  - Features and classification are decoupled

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- Deep learning example.
  - Composition of linear transformations and non-linearities
  - Parametrization of deep models

$$\mathcal{F} : f(x) = \sigma_k(A_k \sigma_{k-1}(A_{k-1} \dots \sigma_2(A_2 \sigma_1(A_1 x))))$$

  - Adaptive features, universal approximation theorem
  - Hard to optimize: non-convex, high-dimensional

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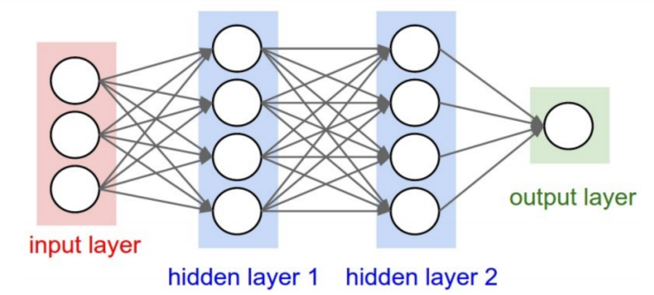

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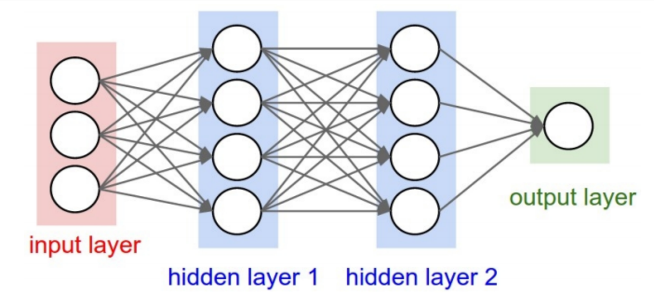

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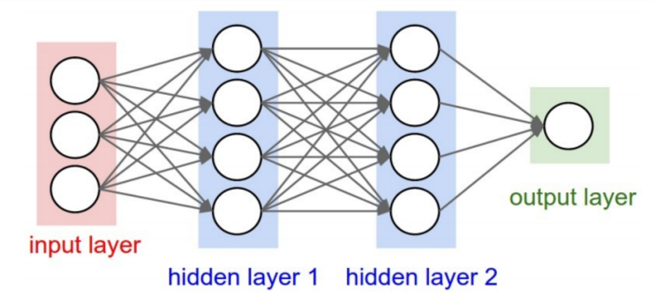

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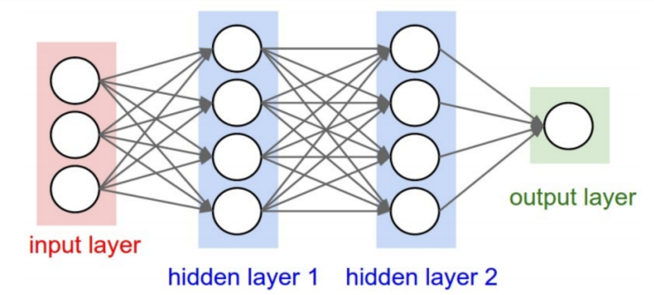

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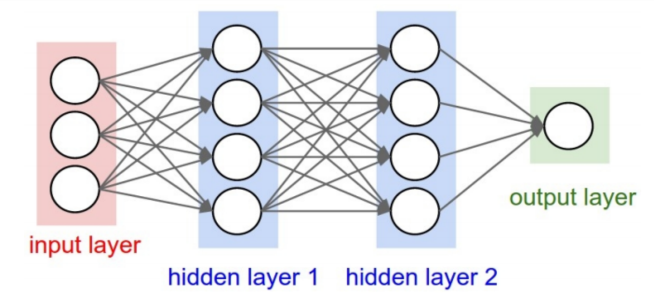

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- Limitations: No invariances, poor scaling of nr parameters

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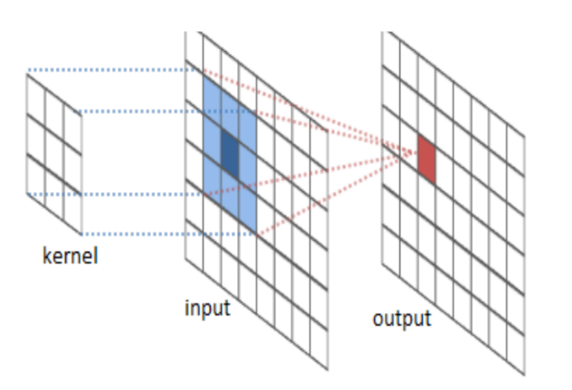

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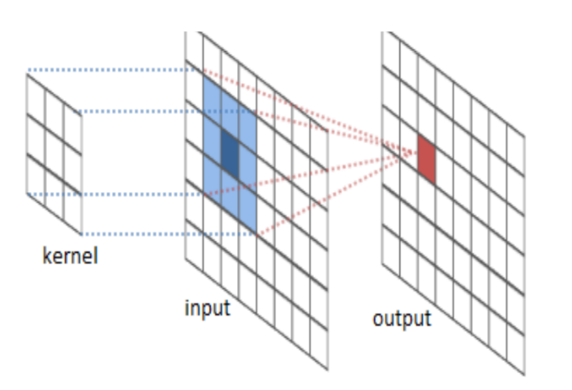

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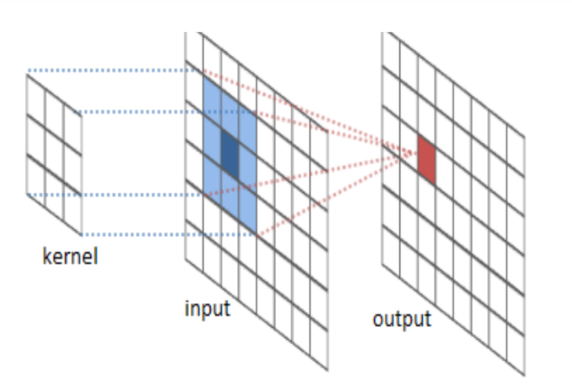

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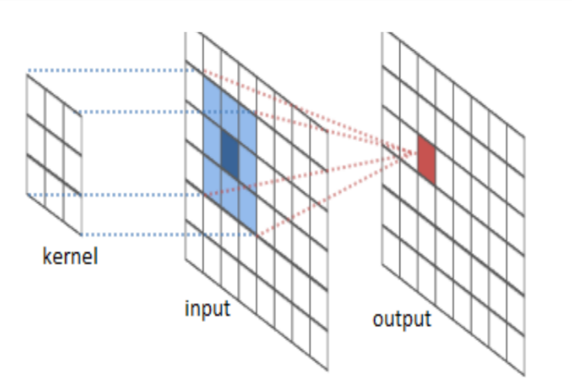

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- Computations single instruction multiple data (SIMD): GPU

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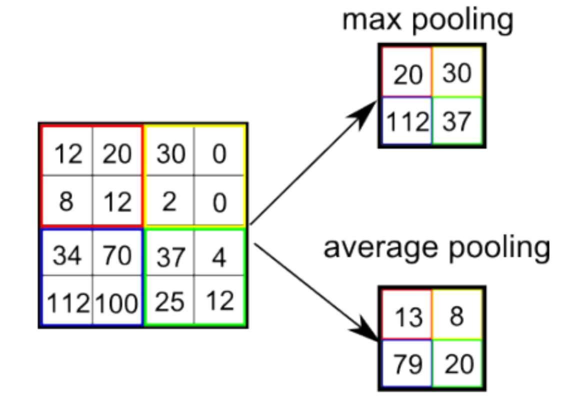

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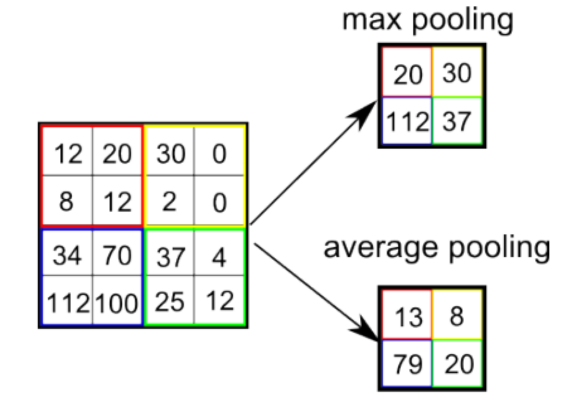

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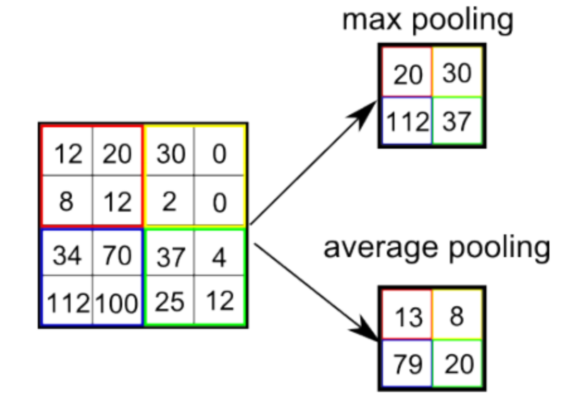

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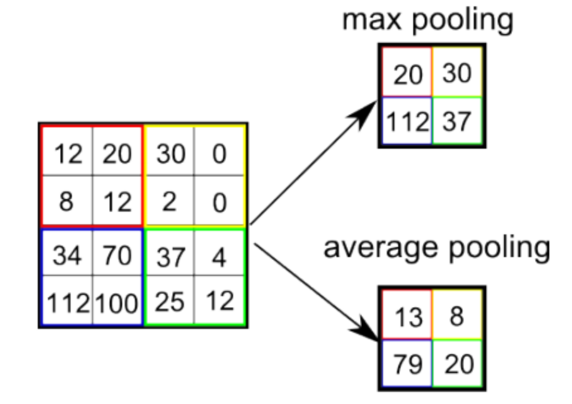
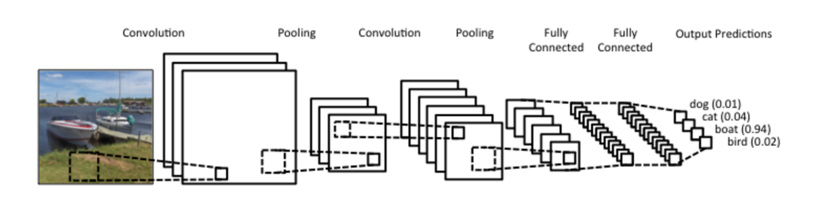


- Reduce spatial dimension
- Increase receptive field
- Or just down-sample after convolution ("strided convolution")

Training deep networks



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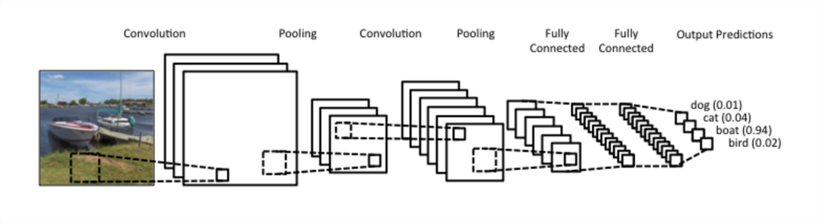

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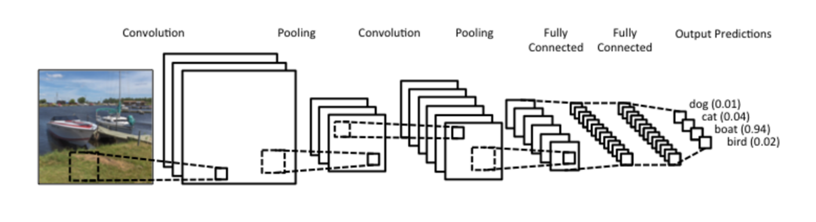

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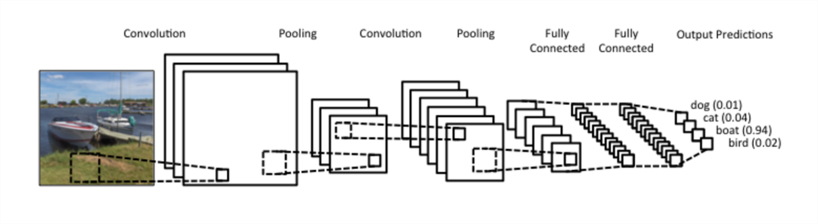

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- Efficient gradient computations via backpropagation algorithm

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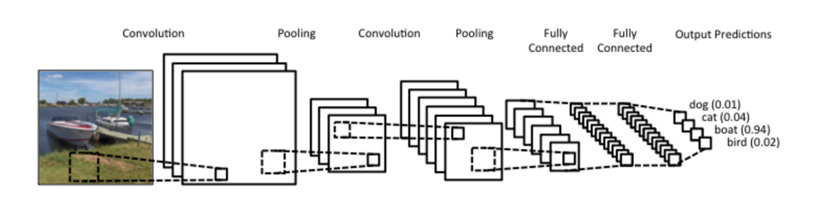

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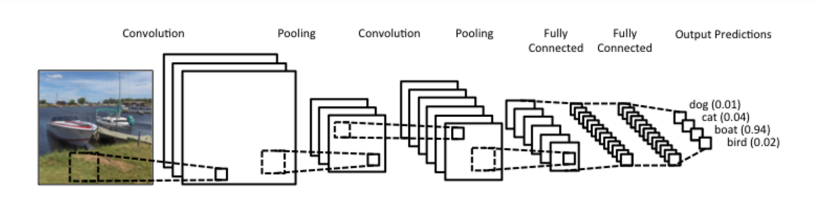

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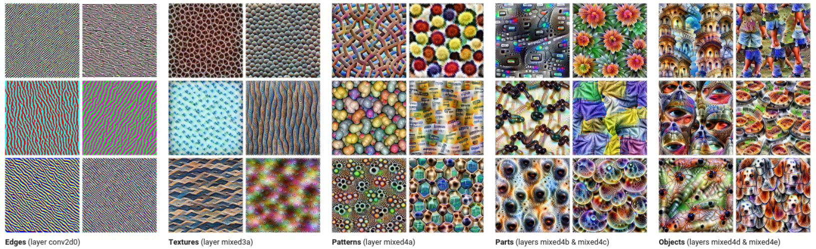

Figure from distill.pub

Take-home messages

- Core idea
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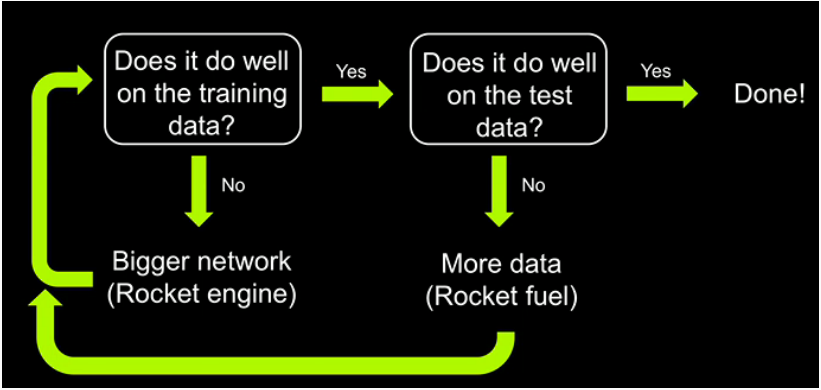
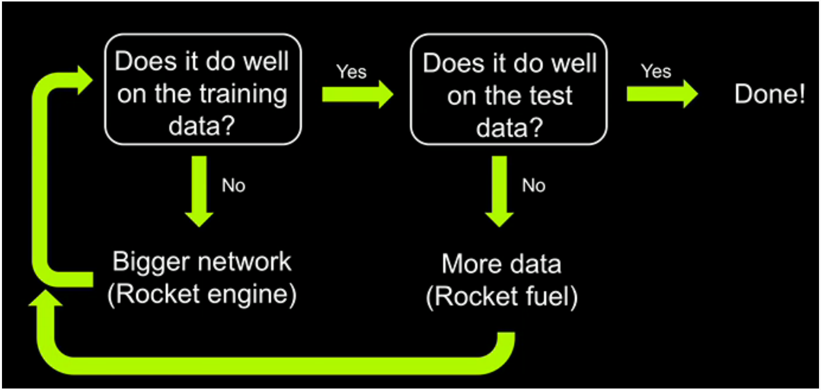
- In theory
    - Optimization still poorly understood
    - Generalization still poorly understood
    - Experimental results 'ahead' of theory

The Limits to Growth



From Andrew Ng's Keynote at Nvidia's GPU Technology Conf. 2015

More labeled data



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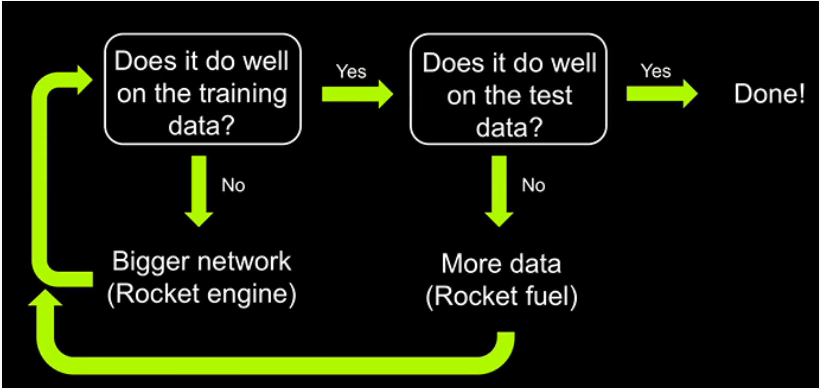
A sustainable approach?



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Part II

Unsupervised deep learning

Motivations for unsupervised deep learning

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   - Conditional density estim. $p_\theta(\mathbf{x}|y)$: text-to-speech, image colorization, video forecasting, **etc**.

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Image colorization [Royer et al., 2017]

Gaussian mixture models

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$$p(\mathbf{x}|z = k) = \mathcal{N}(x; \mu_k, \sigma I_D) \quad (2)$$

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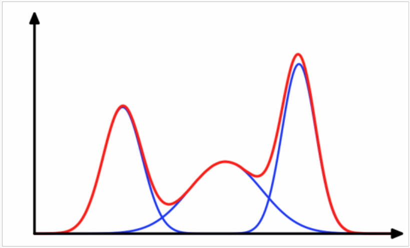

Figure from [Bishop, 2006]

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- Estimation: Expectation-Maximization (EM) algorithm

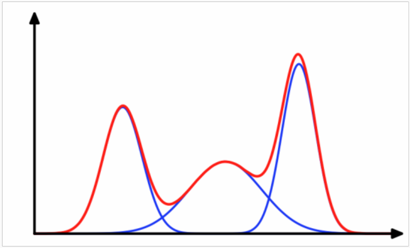

Figure from [Bishop, 2006]

Gaussian mixture models

$$p(z = k) = \pi_k \quad (1)$$

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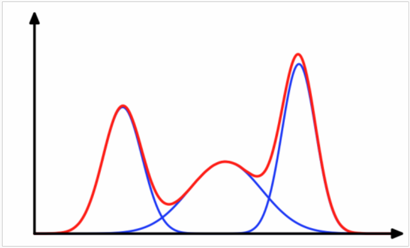

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Linear latent variable models

- Probabilistic Principal Component Analysis [Roweis, 1997, Tipping and Bishop, 1999]

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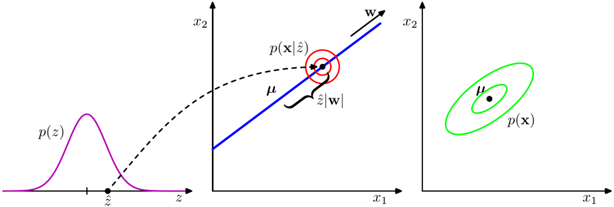

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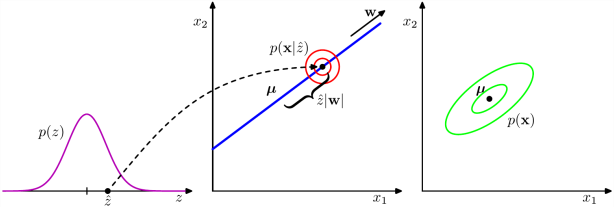

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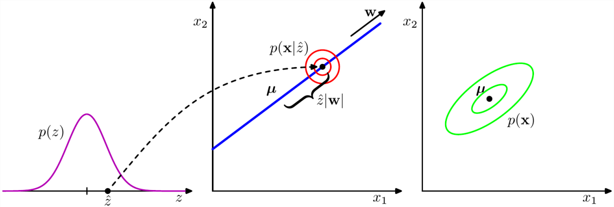

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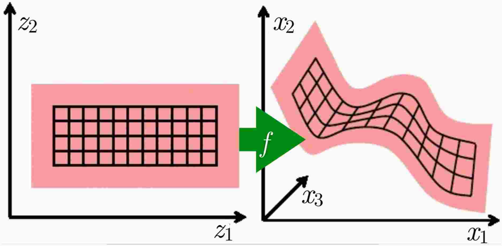

Figure from Aaron Courville

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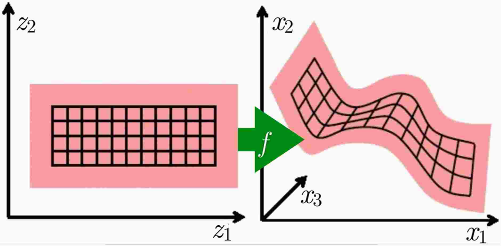

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Learning deep latent variable models

- Marginal distribution on $\mathbf{x}$ obtained by integrating out $\mathbf{z}$

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    - Avoid latent variables: autoregressive models

Part III

Generative adversarial networks

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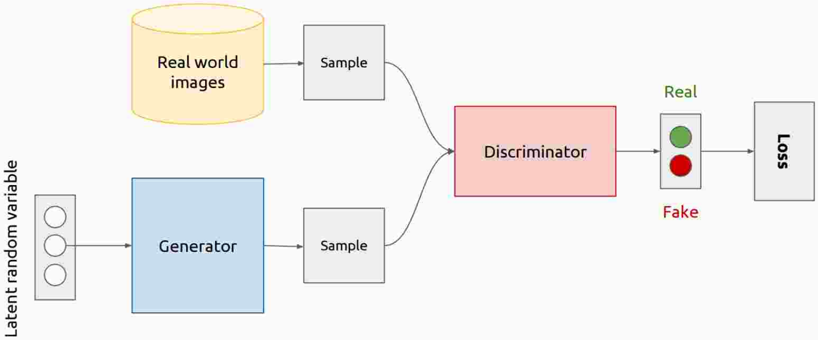

Figure from Kevin McGuinness

Discriminator architecture for images

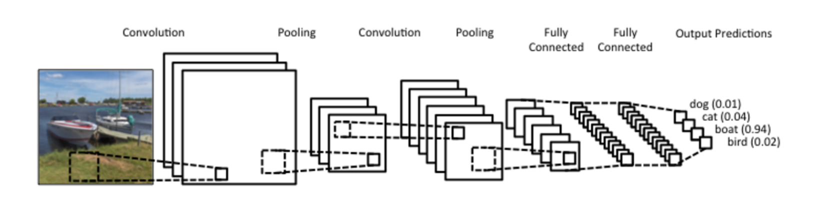

Figure from Kevin McGuinness

- Recognition CNN model, with sigmoid output layer
- Binary classification output: real / synthetic

Generator architecture for images

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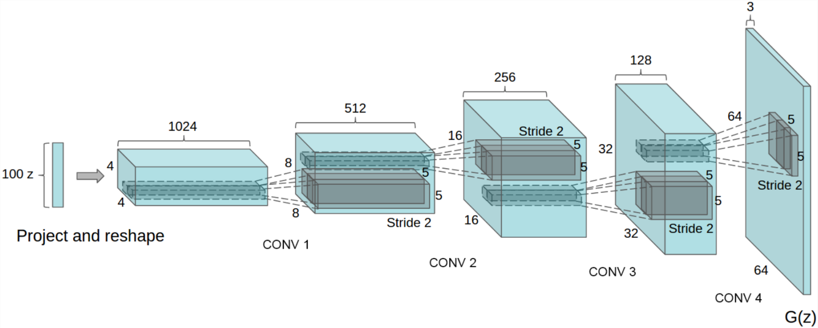

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  - Low-resolution layers induce long-range correlations
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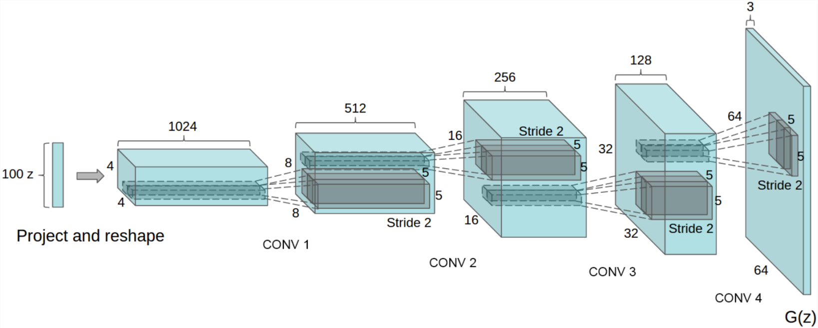

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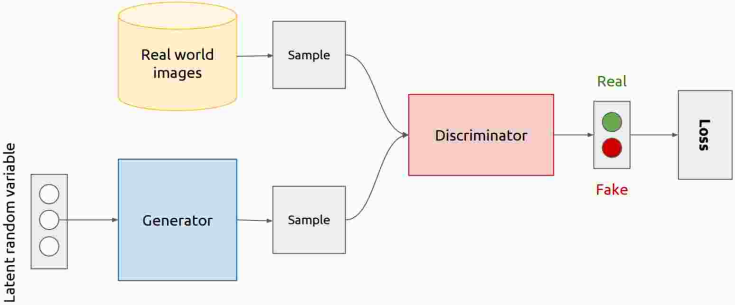
Training GANs



- Discriminator: maximize classification for a given generator
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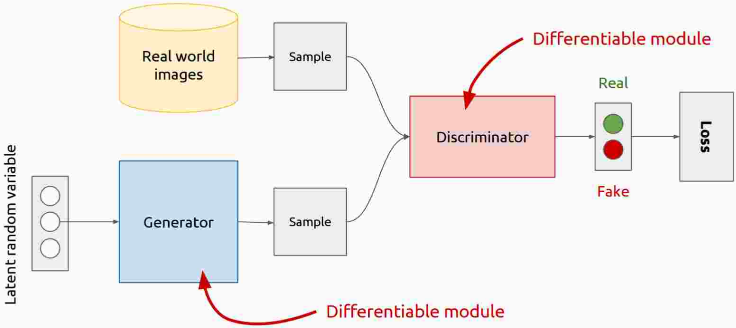

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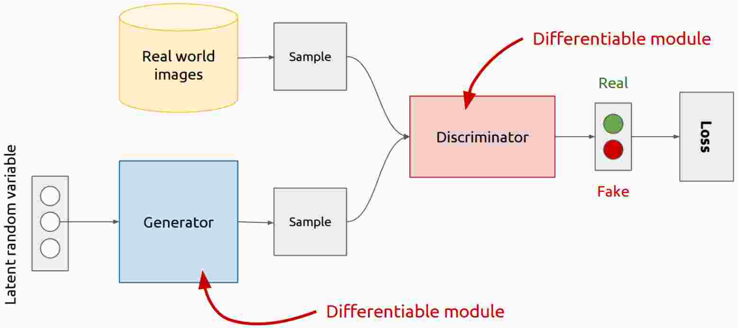

- Discriminator: maximize classification for a given generator
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- Samples **z** pass through two differentiable modules
- Discriminator acts as **trainable loss function**

GAN Optimization problem

- Objective function $V(\phi, \theta)$: performance of discriminator

$$V(\phi, \theta) = \mathbb{E}_{x \sim p_{\mathrm{data}}(x)}[\ln D_\phi(x)] + \mathbb{E}_{x \sim p(\mathbf{z})}[\ln(1 - D_\phi(G_\theta(\mathbf{z})))]$$

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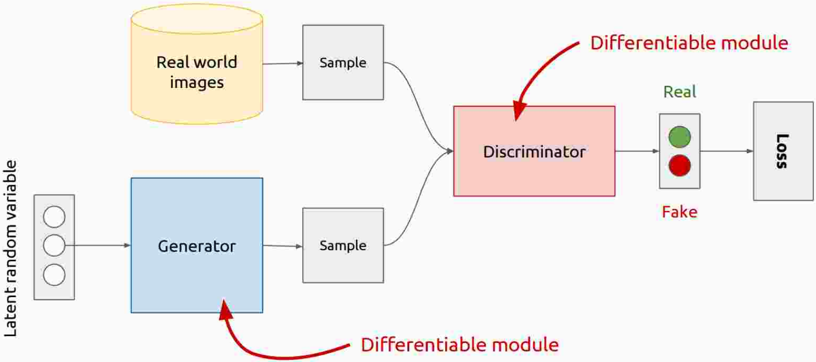
  1. Unique global optimum for G at data distribution
  2. Convergence to optimum guaranteed

Training GANs in practice



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- Replace expectations with sample average in mini-batch

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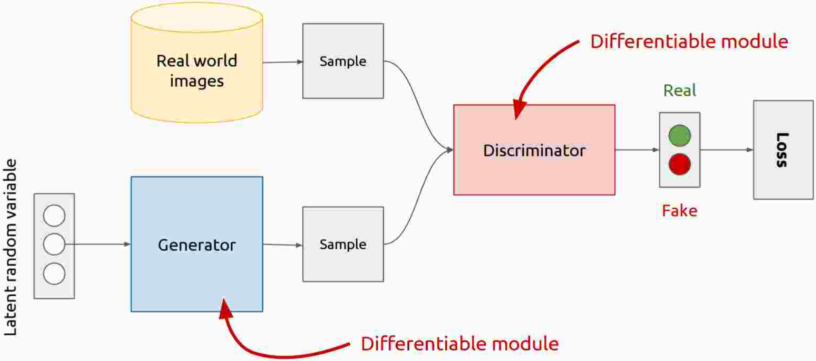

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- Replace expectations with sample average in mini-batch
- Parallel stochastic gradient descent on ϕ and θ

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- GANs known to be difficult to train in practice
  - Formulated as mini-max objective between two networks
  - Optimization can oscillate between solutions
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- Mode collapse: failure to capture parts of training data
  - Optimizes KL-divergence in the "wrong" direction, reverse from MLE [Lucas et al., 2019]

GANs offer outstanding sample quality

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Class conditional ProGan [Karras et al., 2018] samples, for LSUN 256×256

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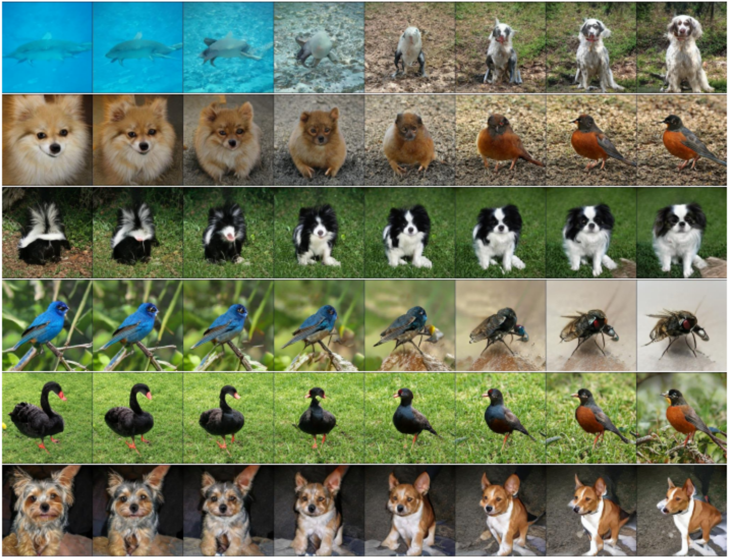


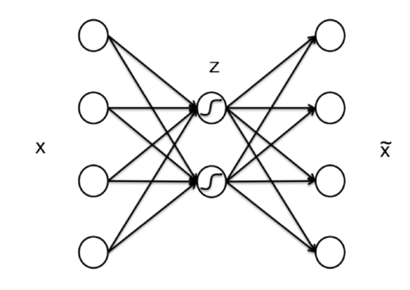
Examples taken from Brock et al. 2019

Part IV

Variational Autoencoders

Autoencoders

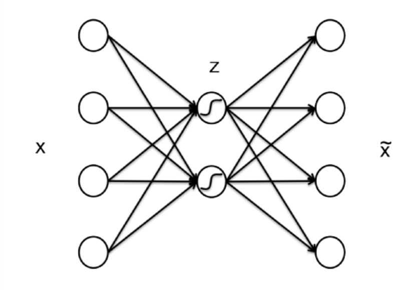
- Learn latent representation **z** via reconstruction of data **x**



Autoencoders

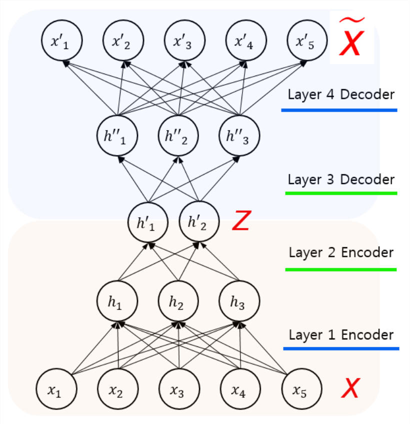
- Learn latent representation **z** via reconstruction of data **x**
- Autoencoder recovers PCA if [Baldi and Hornik, 1989]
  1. Encoder and decoder are both linear
  2. Optimizing ℓ_2 reconstruction loss

$$\min_{V,W} \sum_{n=1}^{N} ||x_n - VWx_n||^2 \tag{9}$$



Deep non-linear autoencoders

- Stack many non-linear layers in encoder and decoder



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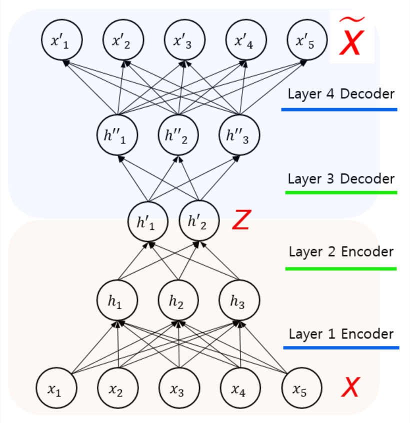
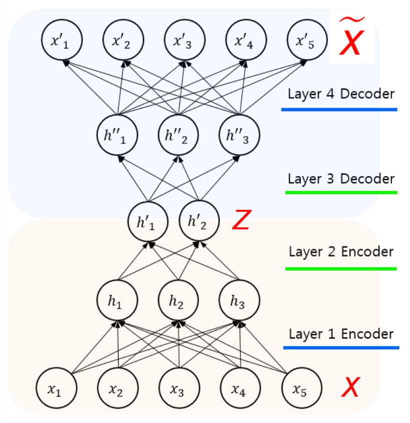


Deep non-linear autoencoders

- Stack many non-linear layers in encoder and decoder
- Non-linear representation learning
- Does not provide a generative model that can be sampled



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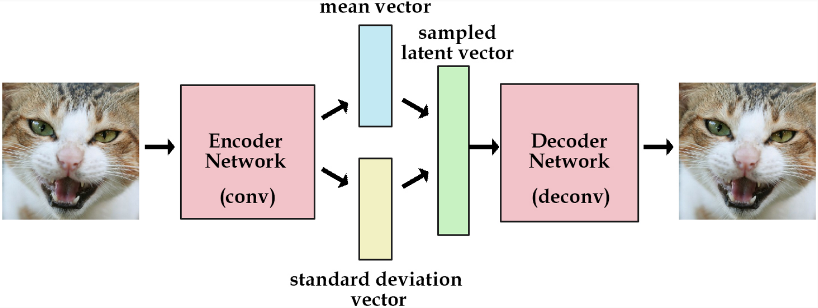

Figure from kvfrans@github

Objective function: Evidence lower bound (ELBO)

- Variational bound on data likelihood using Jensen inequality
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- Optimize both networks jointly with SGD

Computation ELBO for variational autoencoder

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- Differentiable function of inference net parameters

Computation ELBO for variational autoencoder

$$F(\theta, \phi) = \underbrace{\mathbb{E}_{q_\phi}[\ln p_\theta(\mathbf{x}|\mathbf{z})]}_{\textbf{Reconstruction}} - \underbrace{D_{KL}\big(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})\big)}_{\text{Regularization}} \tag{17}$$

- **Reconstruction term**: to what extent can $\mathbf{x}$ be reconstructed from $\mathbf{z}$ following approximate posterior $q(\mathbf{z}|\mathbf{x})$

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- Estimator is non-differentiable due to sampling operator

Re-parametrization trick

- Side-step non-differentiable sampling operator by re-parametrizing samples $\mathbf{z_s} \sim q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}; g_\phi^\mu(\mathbf{x}), g_\phi^\sigma(\mathbf{x})\right)$

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- Use inference net to modulate samples from a unit Gaussian

$$\mathbf{z}_s = g_\phi^\mu(\mathbf{x}) + g_\phi^\sigma(\mathbf{x}) \odot \epsilon_s, \qquad \epsilon_s \sim \mathcal{N}(\epsilon_s; 0, I) \tag{19}$$

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- Unbiased differentiable approximation of ELBO

$$F(\theta, \phi) \approx \frac{1}{S} \sum_{s=1}^{S} \ln p_\theta\left(\mathbf{x}|g_\phi^\mu(\mathbf{x}) + g_\phi^\sigma(\mathbf{x}) \odot \epsilon_s\right) \tag{20}$$

$$-\frac{1}{2}\left[1 + \ln g_\phi^\sigma(\mathbf{x}) - g_\phi^\mu(\mathbf{x}) - g_\phi^\sigma(\mathbf{x})\right] \tag{21}$$

Re-parametrization trick in a cartoon

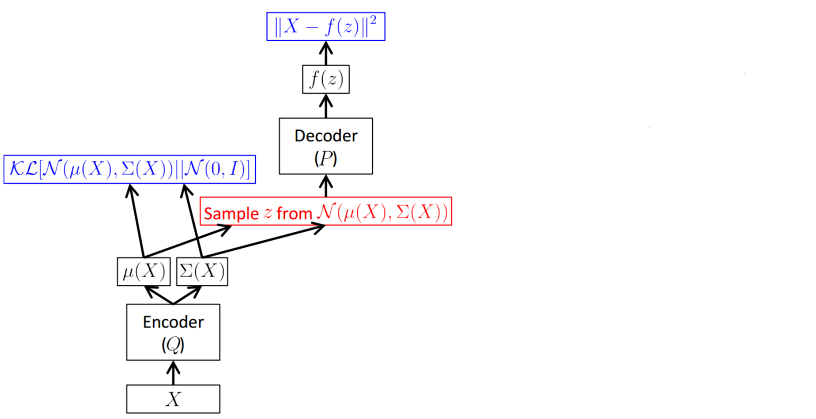

Figure from [Doersch, 2016]

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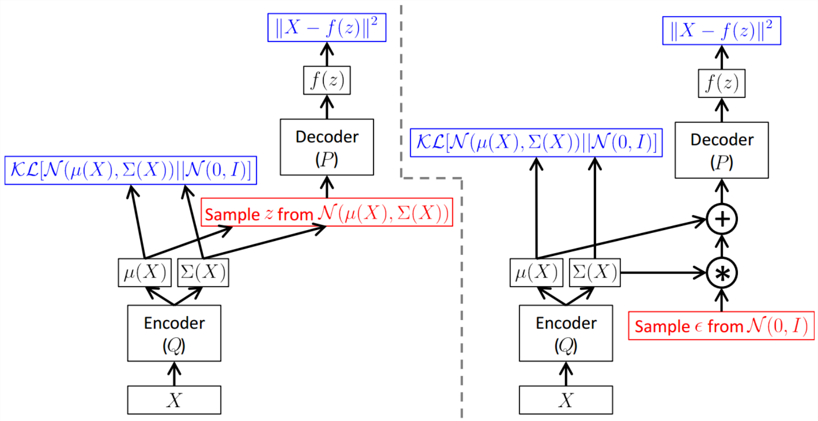

Figure from [Doersch, 2016]

Autoencoding variational Bayes training algorithm

- For each data point $\mathbf{x}$ in a mini-batch
  1. Sample one or multiple values $\{\epsilon_s\}$
  2. Use back-propagation to compute
     $g_\theta = \nabla_\theta F(\theta, \phi, \{\epsilon_s\})$
     $g_\phi = \nabla_\phi F(\theta, \phi, \{\epsilon_s\})$
  3. Gradient-based parameter update

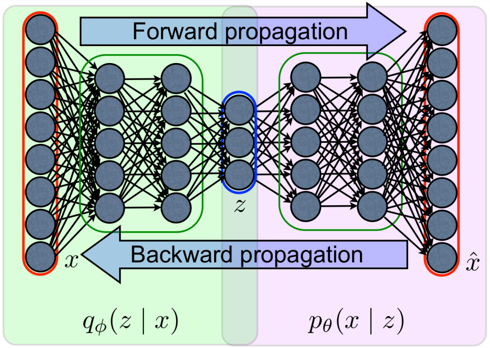

Figure from Aaron Courville

VAE compared to GAN

- VAE does not suffer from GAN training instability
- GANs typically have higher sample quality than VAE
- VAE defines likelihood $p(\mathbf{x})$ for all data $\mathbf{x}$,
  can **e.g**. be used for loss-less compression

Figure from [Hou et al., 2017], models trained on CelebA dataset

Part V

Deep invertible transformations

Modeling via the change of variable formula

- Learn invertible "flow", $f(\cdot)$, between latent and data space

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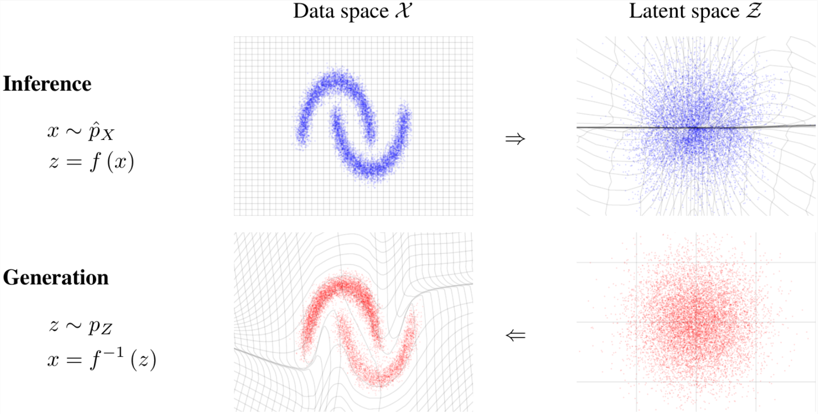

Figure from [Dinh et al., 2017]

Change of variables formula for invertible function

- Express density estimation in latent space

$$
\begin{aligned}
\mathbf{y} &= f(\mathbf{x}), && (22)\\
J_f &= \frac{\partial \mathbf{y}}{\partial \mathbf{x}^\top}, && (23)\\
p_X(\mathbf{x}) &= p_Y(\mathbf{y}) \times |\det(J_f)| && (24)
\end{aligned}
$$

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- Sampling: $\mathbf{y} \sim p(\mathbf{y})$, map through inverse $\mathbf{x} = f^{-1}(\mathbf{y})$

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- Impose structure on $f(\cdot)$ to make both operations efficient

Non-volume Preserving transformations (NVP) [Dinh et al., 2017]

- Stack many invertible "coupling layers"
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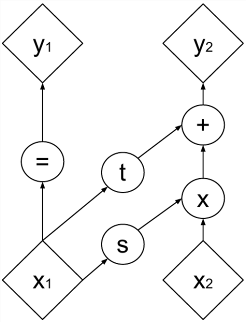
   For example, half of pixels in one group



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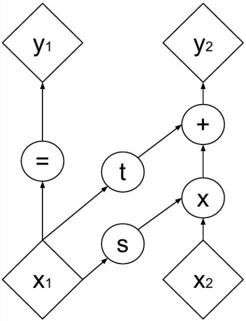

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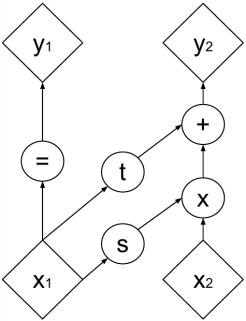
   For example, half of pixels in one group

2. Keep group $\mathbf{x}_1$ unchanged

3. Let $\mathbf{x}_1$ transform $\mathbf{x}_2$ via translation and scaling

$$\begin{aligned} \mathbf{y}_1 &= \mathbf{x}_1 \\ \mathbf{y}_2 &= t(\mathbf{x}_1) + \mathbf{x}_2 \odot \exp(s(\mathbf{x}_1)) \end{aligned}$$



Properties: Efficient inversion

- Inverse transformation

$$\mathbf{x}_1 = \mathbf{y}_1 \tag{25}$$

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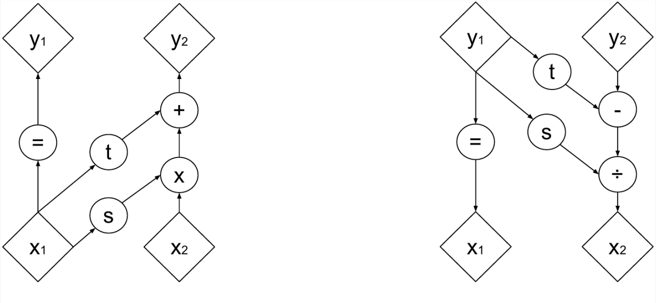

(a) Forward propagation (b) Inverse propagation

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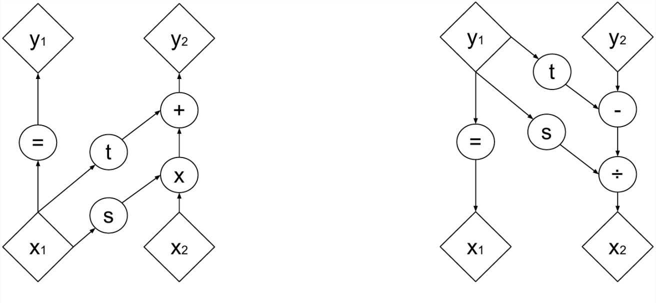
- No need to invert $s(\cdot)$ and $t(\cdot)$
- Can use complex non-invertible functions, **e.g**. deep CNN



(a) Forward propagation (b) Inverse propagation

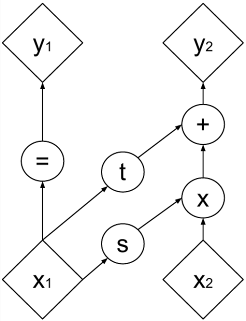
Properties: Efficient determinant computation

- Triangular structure of Jacobian

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}^\top} = \begin{bmatrix} I_d & 0 \\ \frac{\partial \mathbf{y}_2}{\partial \mathbf{x}_1^\top} & \mathrm{diag}(\exp(s(\mathbf{x}_1))) \end{bmatrix}$$

- Determinant given by product of Jacobian's diagonal terms

$$\ln \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}^\top} \right) \right| = \mathbf{1}^\top s(\mathbf{x}_1)$$



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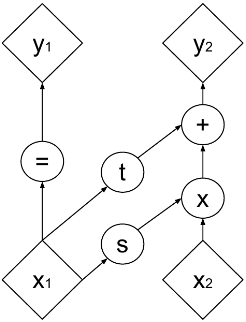
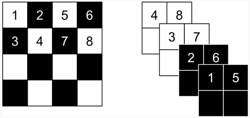
- Log-likelihood easily computed, optimize using stochastic gradient decent

$$\ln p_X(\mathbf{x}) = \ln p_Y(f(\mathbf{x})) + \mathbf{1}^\top s(\mathbf{x}_1)$$



Implementation

- Layers cycle through various partitionings
  - Checkerboard mask
  - Channel-wise mask



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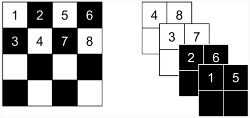

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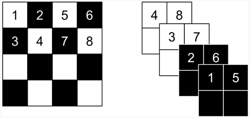
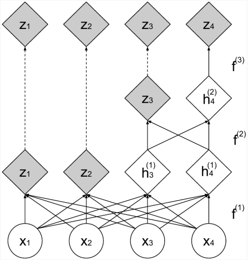


- Multi-scale architecture
  - Down sample at regular intervals



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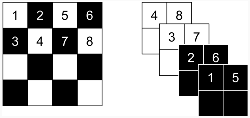
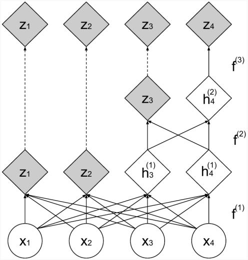
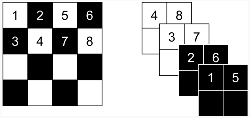


- Multi-scale architecture
  - Down sample at regular intervals
  - Squeeze $2h \times 2w \times c$ map into $h \times w \times 4c$





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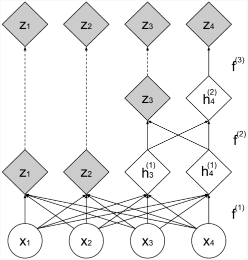
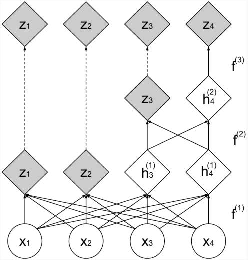


- Multi-scale architecture
  - Down sample at regular intervals
  - Squeeze $2h \times 2w \times c$ map into $h \times w \times 4c$
  - "Freeze" half the channels / latent vars.

Illustration multi-scale feature hierarchy

- Images obtained after re-sampling part of latent variables



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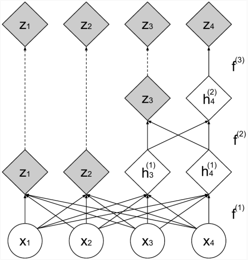
- From left to right: original, keeping $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}$

ImageNet 64×64



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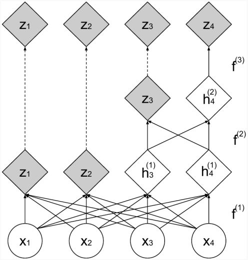
CelebA 64×64



Flow vs. VAE & GAN

- Flow offers stable training ($\neq$GAN) with exact likelihood ($\neq$VAE)
- VAE offers best likelihood on held-out data
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Samples from flow model trained on CelebA 256$\times$256 [Kingma and Dhariwal, 2018]

Part VI

Autoregressive density estimation

Autoregressive modeling

- Avoid intractable integral over latent variables

Autoregressive modeling

- Avoid intractable integral over latent variables
- Consider generic factorization of joint probability

$$p(\mathbf{x}_{1:D}) = p(x_1) \prod_{i=2}^{D} p(x_i | \mathbf{x}_{<i}) \tag{27}$$

with $\mathbf{x}_{<i} = \mathbf{x}_1, \ldots, \mathbf{x}_{i-1}$

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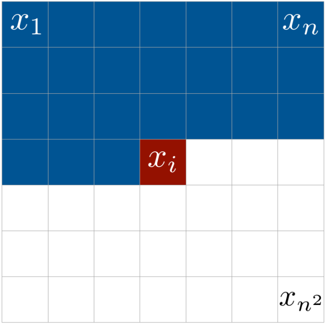
  with $\mathbf{x}_{<i} = \mathbf{x}_1, \ldots, \mathbf{x}_{i-1}$
- Use deep neural net to model complex conditionals $p(x_i|\mathbf{x}_{<i})$
- Tractable exact likelihood computations
- Slow sequential one-by-one sampling of pixels
  - Cannot rely on latent variables to induce dependencies

Pixel Convolutional Neural Networks [Oord et al., 2016a]

- Predict pixels one-by-one in row-major ordering



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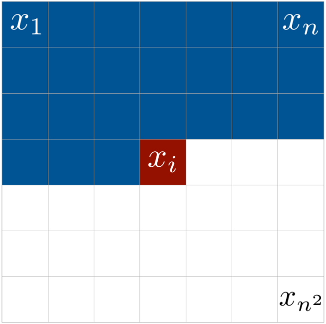
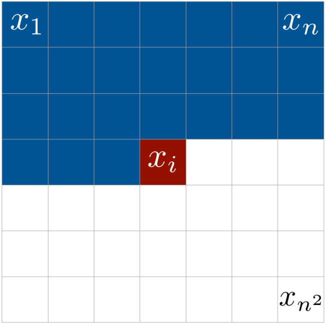
- Translation invariant definition of conditionals $p(x_i|\mathbf{x}_{<i})$



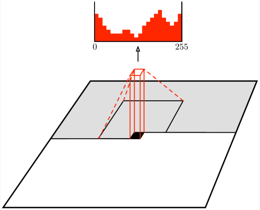
Pixel Convolutional Neural Networks [Oord et al., 2016a]

- Predict pixels one-by-one in row-major ordering
- Translation invariant definition of conditionals $p(x_i|\mathbf{x}_{<i})$
- Decouple number of pixels from number of parameters



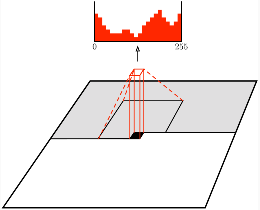
Pixel Convolutional Neural Networks

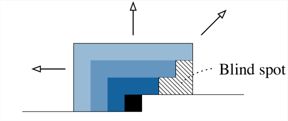
- Use limited context via CNN layers
    - Only local dependencies per layer
- Masked convolutions to ensure autoregressive property



Pixel Convolutional Neural Networks

- Use limited context via CNN layers
  - Only local dependencies per layer
  - Adding layers increases context
- Masked convolutions to ensure autoregressive property





Pixel Convolutional Neural Networks

- Use limited context via CNN layers
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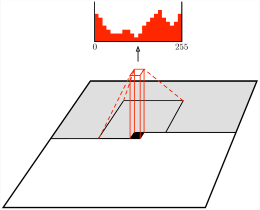
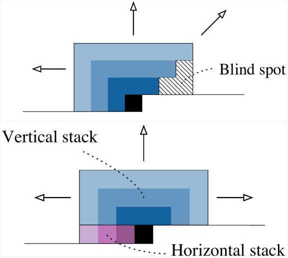
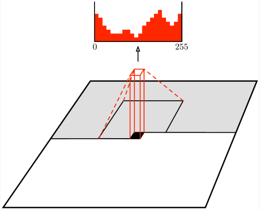
- Masked convolutions to ensure autoregressive property
  - Block pixels below / right

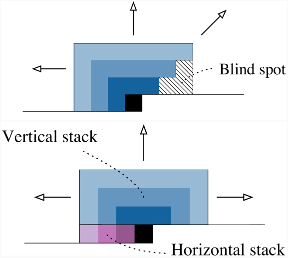




Pixel Convolutional Neural Networks

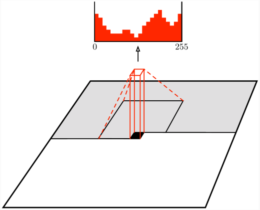
- Use limited context via CNN layers
  - Only local dependencies per layer
  - Adding layers increases context
- Masked convolutions to ensure autoregressive property
  - Block pixels below / right
  - Blind spot filled using two feature stacks

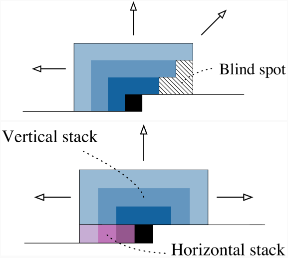




Pixel Convolutional Neural Networks

- Use limited context via CNN layers
  - Only local dependencies per layer
  - Adding layers increases context
- Masked convolutions to ensure autoregressive property
  - Block pixels below / right
  - Blind spot filled using two feature stacks
- Efficient parallel training, sampling remains slow





WaveNet: Autoregressive audio model

- Autoregressive CNN model in 1 dimension of raw waveform

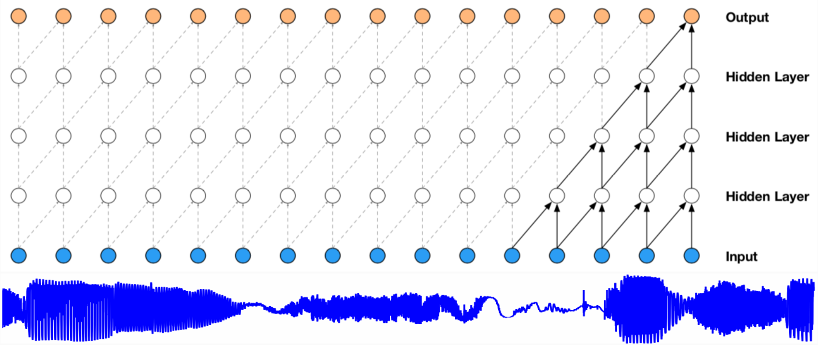


Figure from [Kalchbrenner et al., 2017]

Multiscale autoregressive modeling [Reed et al., 2017]

- Address the inherently limited sampling efficiency of autoregressive models

$$p(\mathbf{x}_{1:N}) = \prod_{i=1}^{N} p(x_i | \mathbf{x}_{<i})$$

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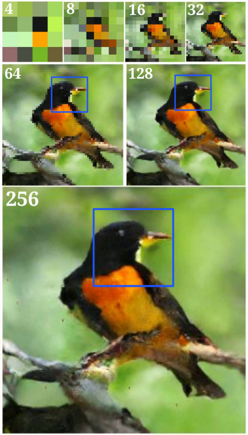
- Sample image along a scale pyramid
  - Pixel-CNN for base resolution, **e.g**. 4×4
  - Autoregressive upsampling networks



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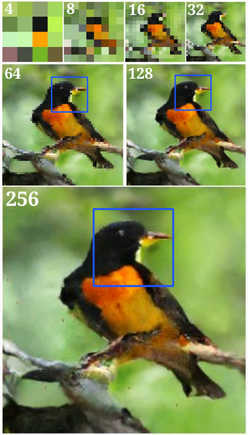
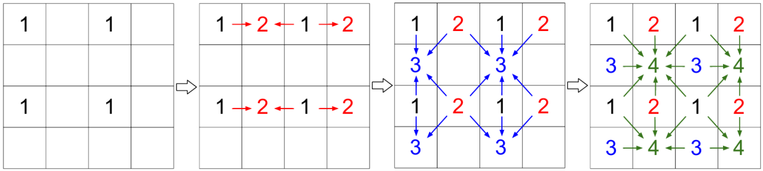
- Sample image along a scale pyramid
  - Pixel-CNN for base resolution, **e.g**. 4×4
  - Autoregressive upsampling networks
- Impose group structure among pixels
  - Sample independent within group
  - Sample autoregressive across groups



Sampling pixels in groups

- Group pixels along position in 2×2 blocks
  - Group 1 given from previous resolution
  - Sample remaining pixels in three steps



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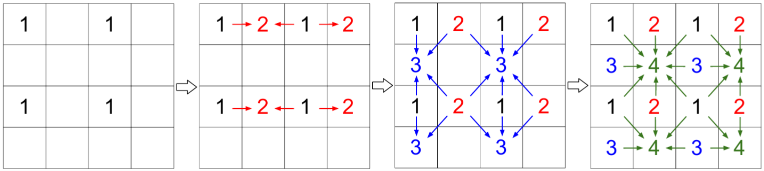
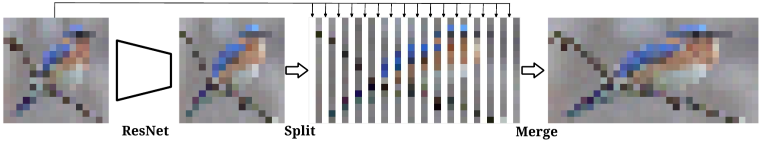


- Example network to predict group 2 from group 1
  - Use CNN without pooling to predict/sample new columns
  - Interleave pixel columns from group 1 and 2



Example results of upsampling real low-resolution images

- About 100× speed-up w.r.t. pixel-CNN sampling

Pixel CNN compared to VAE and GAN

- Exact likelihoods unlike VAE and GAN

Class-conditional pixelCNN 32×32 samples trained on ImageNet [Oord et al., 2016b]

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- Convincing samples at low resolutions, too slow for high resolution

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  - No need for labeled training data!
  - Semi-supervised learning, prediction of missing data, ...
  - Generation of realistic (and varied) samples of speech, images, ...

Thanks for your attention!

Jakob Verbeek
INRIA, Grenoble, France

jakob.verbeek@inria.fr

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