Deep Learning
Unsupervised Learning

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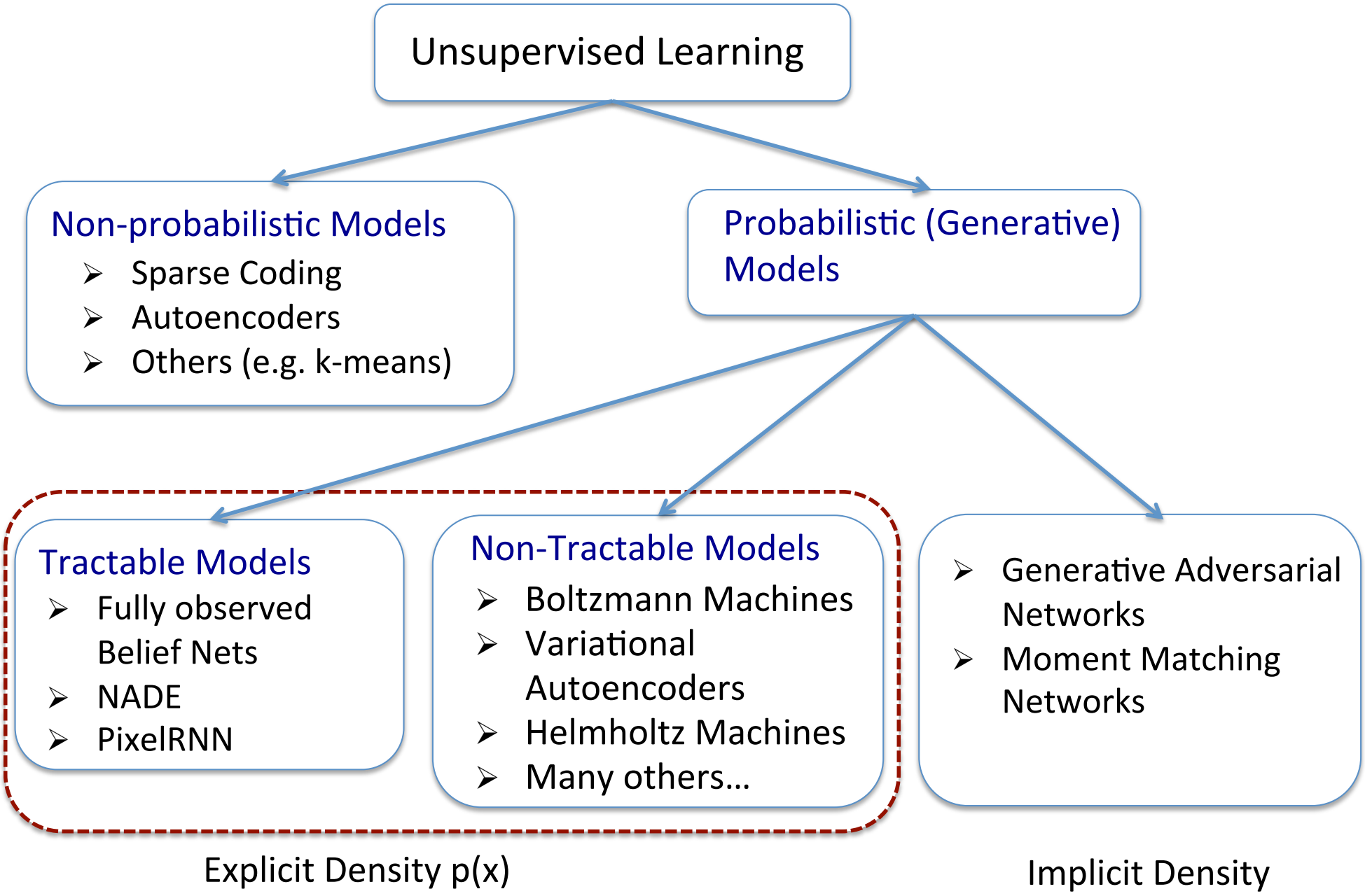
Tutorial Roadmap

Part 1: Supervised (Discriminative) Learning: Deep Networks

Part 2: Unsupervised Learning: Deep Generative Models

Part 3: Open Research Questions


Unsupervised Learning
Non-probabilistic Models
Sparse Coding
Autoencoders
Others (e.g. k-means)
Probabilistic (Generative) Models
Tractable Models
Fully observed Belief Nets
NADE
PixelRNN
Non-Tractable Models
Boltzmann Machines
Variational Autoencoders
Helmholtz Machines
Many others…
Generative Adversarial Networks
Moment Matching Networks
Explicit Density p(x)
Implicit Density

Tutorial Roadmap

- Basic Building Blocks:
  - Sparse Coding
  - Autoencoders
- Deep Generative Models
  - Restricted Boltzmann Machines
  - Deep Boltzmann Machines
  - Helmholtz Machines / Variational Autoencoders
- Generative Adversarial Networks

Tutorial Roadmap

- Basic Building Blocks:
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Sparse Coding

• Sparse coding (Olshausen & Field, 1996). Originally developed to explain early visual processing in the brain (edge detection).

• Objective: Given a set of input data vectors $\{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$, learn a dictionary of bases $\{\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, ..., \boldsymbol{\phi}_K\}$, such that:

$$\mathbf{x}_n = \sum_{k=1}^{K} a_{nk}\boldsymbol{\phi}_k,$$

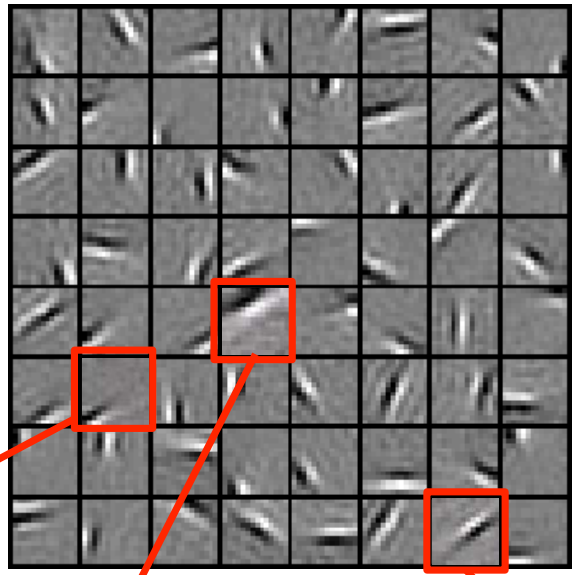
Sparse: mostly zeros

• Each data vector is represented as a sparse linear combination of bases.

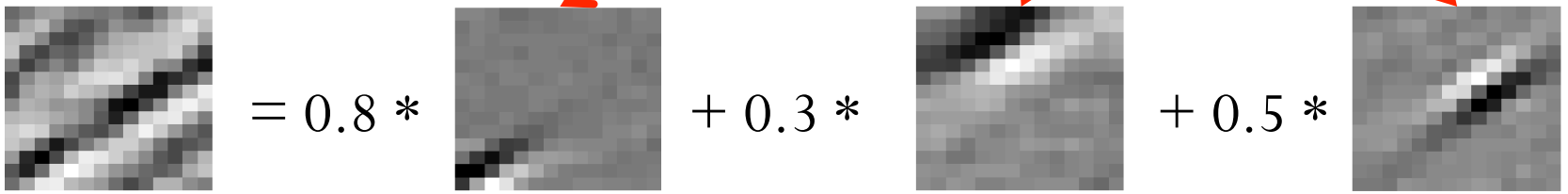
Sparse Coding

Natural Images

Learned bases: "Edges"



New example



$$x = 0.8 * \phi_{36} + 0.3 * \phi_{42} + 0.5 * \phi_{65}$$

[0, 0, … **0.8**, …, **0.3**, …, **0.5**, …] = coefficients (feature representation)

Slide Credit: Honglak Lee

Sparse Coding: Training

- Input image patches: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \mathbb{R}^D$
- Learn dictionary of bases: $\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_K \in \mathbb{R}^D$

$$\min_{\mathbf{a},\boldsymbol{\phi}} \sum_{n=1}^{N} \left\| \mathbf{x}_n - \sum_{k=1}^{K} a_{nk}\boldsymbol{\phi}_k \right\|_2^2 + \lambda \sum_{n=1}^{N}\sum_{k=1}^{K} |a_{nk}|$$

Reconstruction error Sparsity penalty

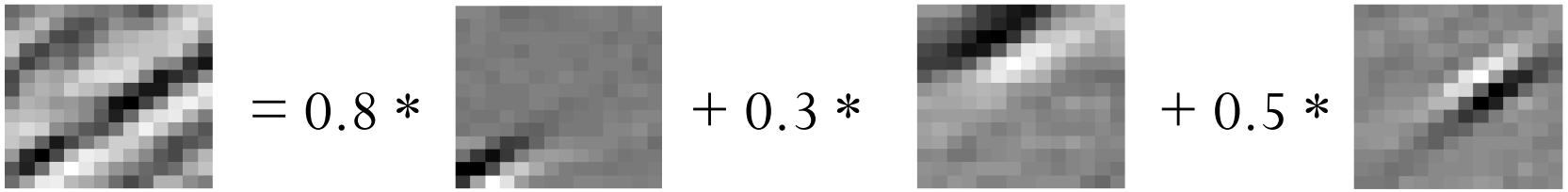
- Alternating Optimization:

1. Fix dictionary of bases $\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_K$ and solve for activations **a** (a standard Lasso problem).
2. Fix activations **a**, optimize the dictionary of bases (convex QP problem).

Sparse Coding: Testing Time

- Input: a new image patch x* , and K learned bases $\phi_1, \phi_2, ..., \phi_K$
- Output: sparse representation **a** of an image patch x*.

$$\min_{\mathbf{a}} \left\| \mathbf{x}^* - \sum_{k=1}^{K} a_k \phi_k \right\|_2^2 + \lambda \sum_{k=1}^{K} |a_k|$$

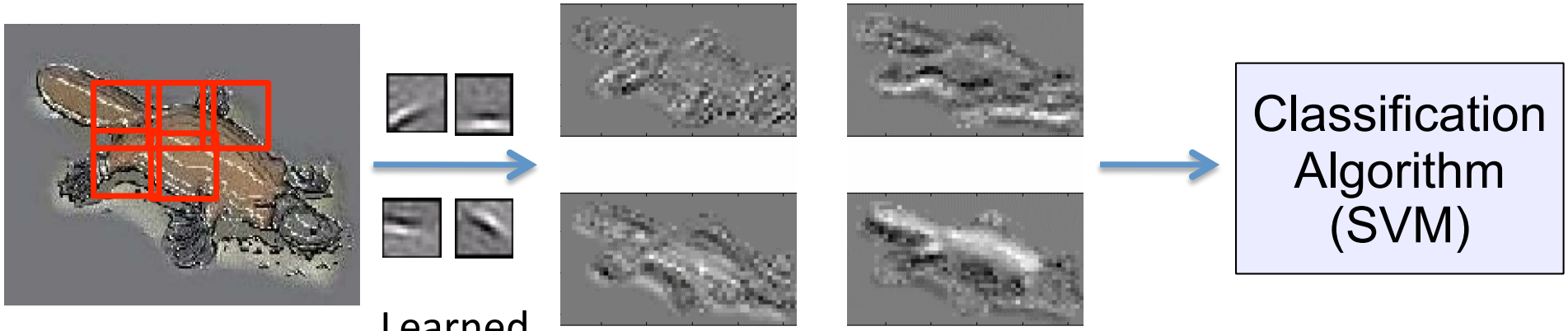


x^* $= 0.8 *$ ϕ_{36} $+ 0.3 *$ ϕ_{42} $+ 0.5 *$ ϕ_{65}

[0, 0, … **0.8**, …, **0.3**, …, **0.5**, …] = coefficients (feature representation)

Image Classification

Evaluated on Caltech101 object category dataset.

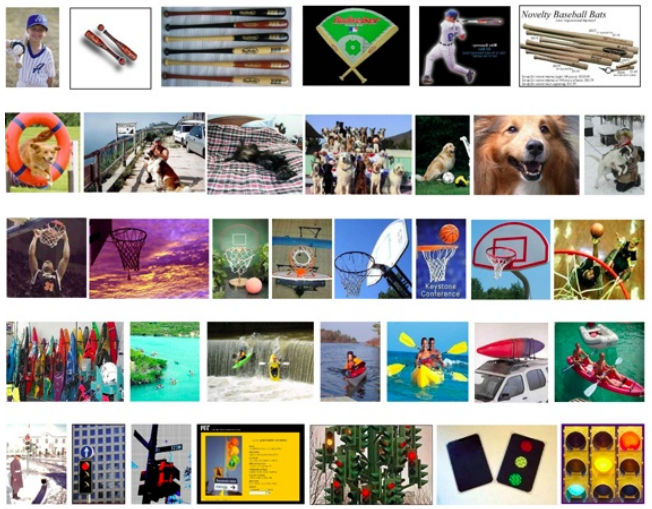


Input Image

Learned bases

Features (coefficients)

9K images, 101 classes



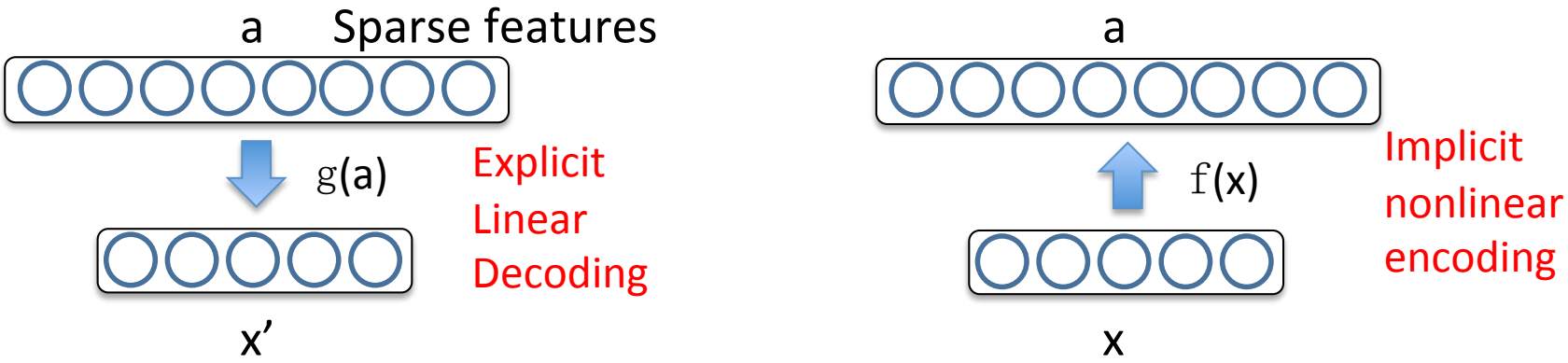
Algorithm	Accuracy
Baseline (Fei-Fei et al., 2004)	16%
PCA	37%
Sparse Coding	**47%**

Slide Credit: Honglak Lee

Lee, Battle, Raina, Ng, 2006

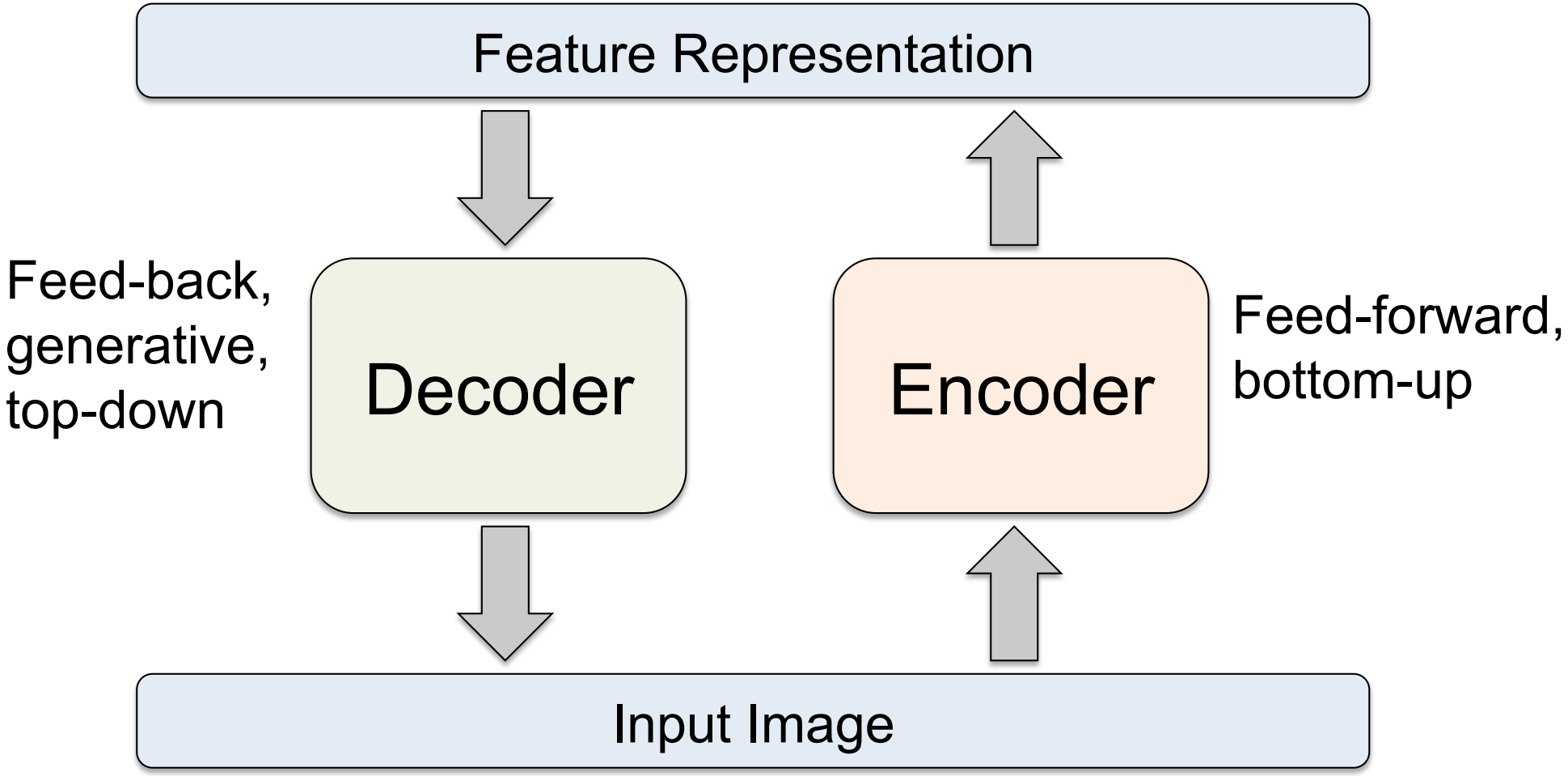
Interpreting Sparse Coding

$$\min_{\mathbf{a},\boldsymbol{\phi}} \sum_{n=1}^{N} \left|\left| \mathbf{x}_n - \sum_{k=1}^{K} a_{nk}\boldsymbol{\phi}_k \right|\right|_2^2 + \lambda \sum_{n=1}^{N}\sum_{k=1}^{K} |a_{nk}|$$



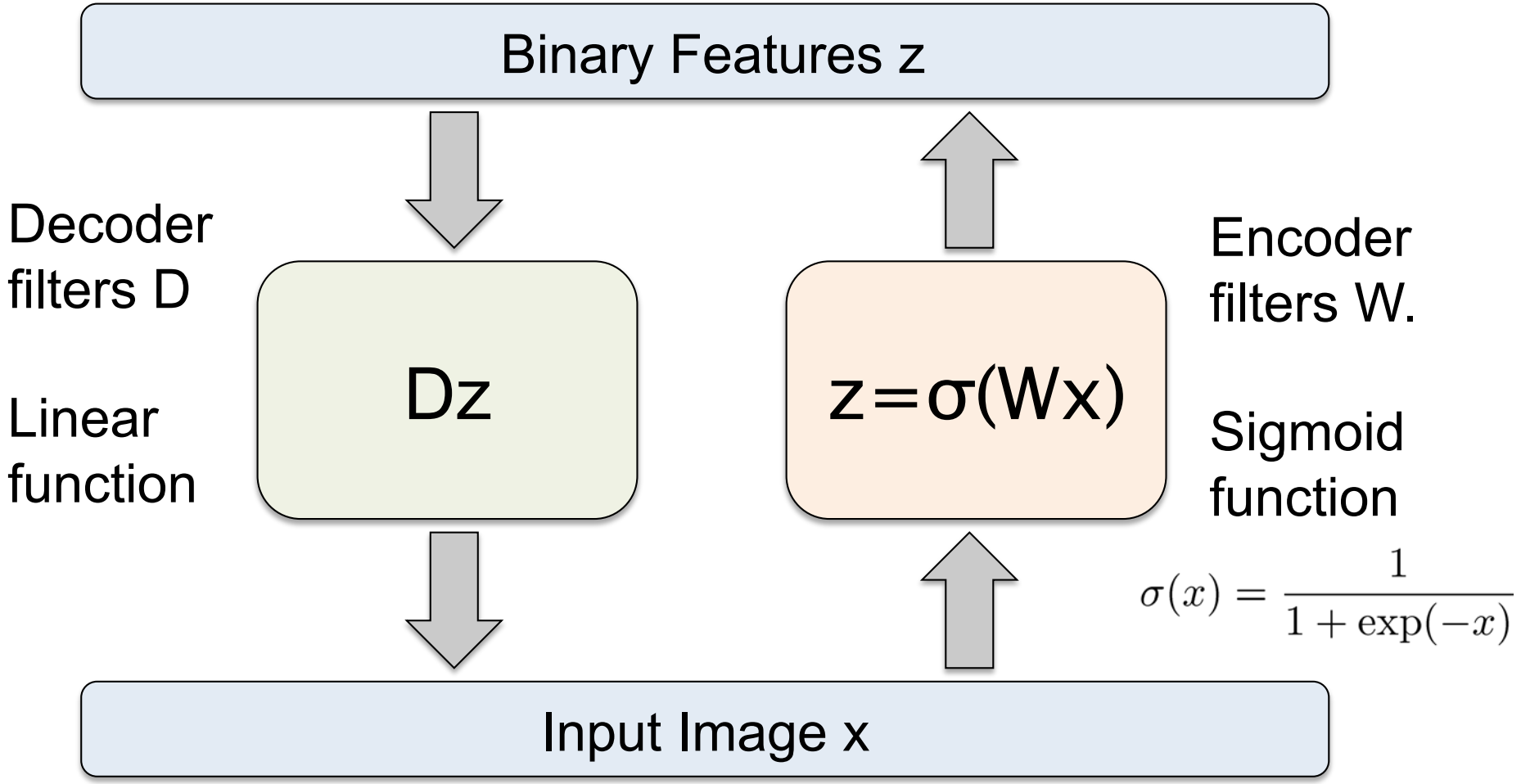
- Sparse, over-complete representation **a.**
- Encoding **a** = f(**x**) is implicit and nonlinear function of **x**.
- Reconstruction (or decoding) **x'** = g(**a**) is linear and explicit.

Autoencoder

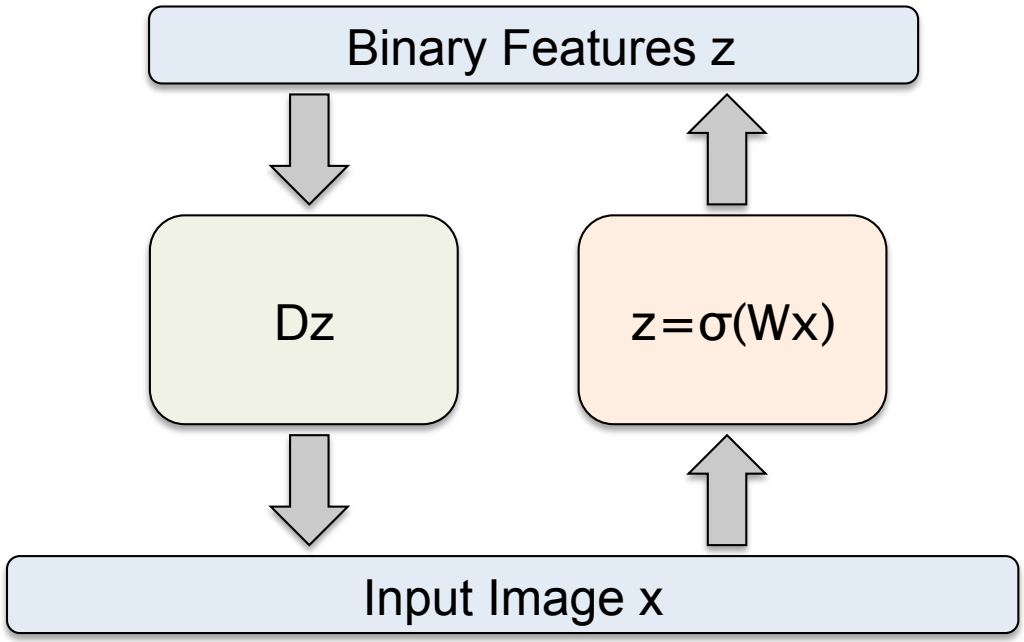


- Details of what goes insider the encoder and decoder matter!
- Need constraints to avoid learning an identity.

Autoencoder



Autoencoder



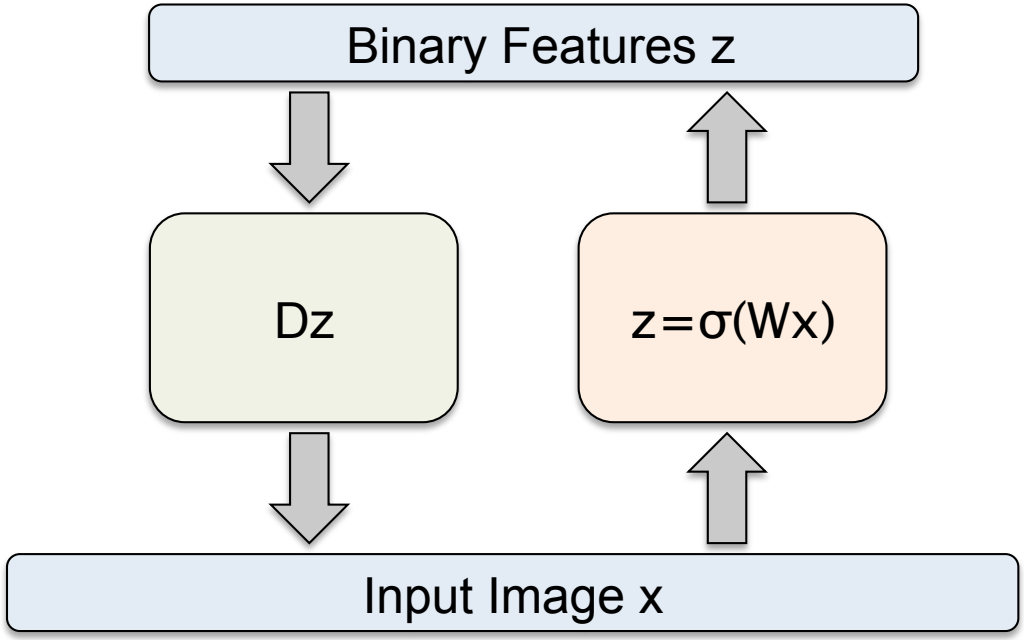
- An autoencoder with D inputs, D outputs, and K hidden units, with K<D.

- Given an input x, its reconstruction is given by:

$$y_j(\mathbf{x}, W, D) = \underbrace{\sum_{k=1}^{K} D_{jk}}_{\text{Decoder}} \underbrace{\sigma\left(\sum_{i=1}^{D} W_{ki} x_i\right)}_{\text{Encoder}}, \quad j = 1, .., D.$$

$$y_j = \sum_{k=1}^{K} D_{jk} z_k \qquad z_k = \sigma\left(\sum_{i=1}^{D} W_{ki} x_i\right)$$

Autoencoder

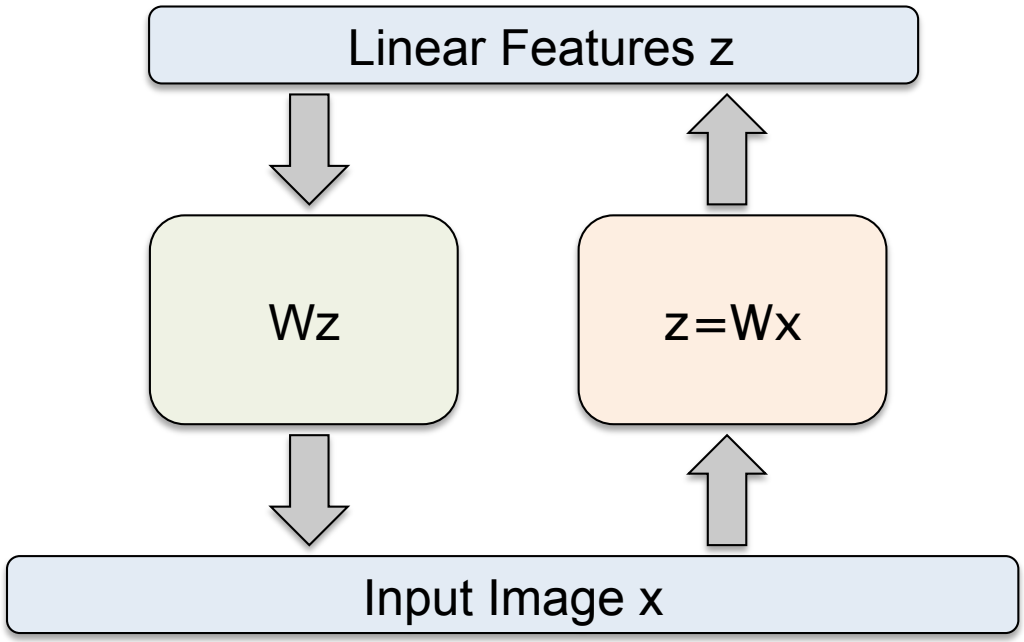


• An autoencoder with D inputs, D outputs, and K hidden units, with K<D.

• We can determine the network parameters W and D by minimizing the reconstruction error:

$$E(W, D) = \frac{1}{2} \sum_{n=1}^{N} ||y(\mathbf{x}_n, W, D) - \mathbf{x}_n||^2.$$

Autoencoder

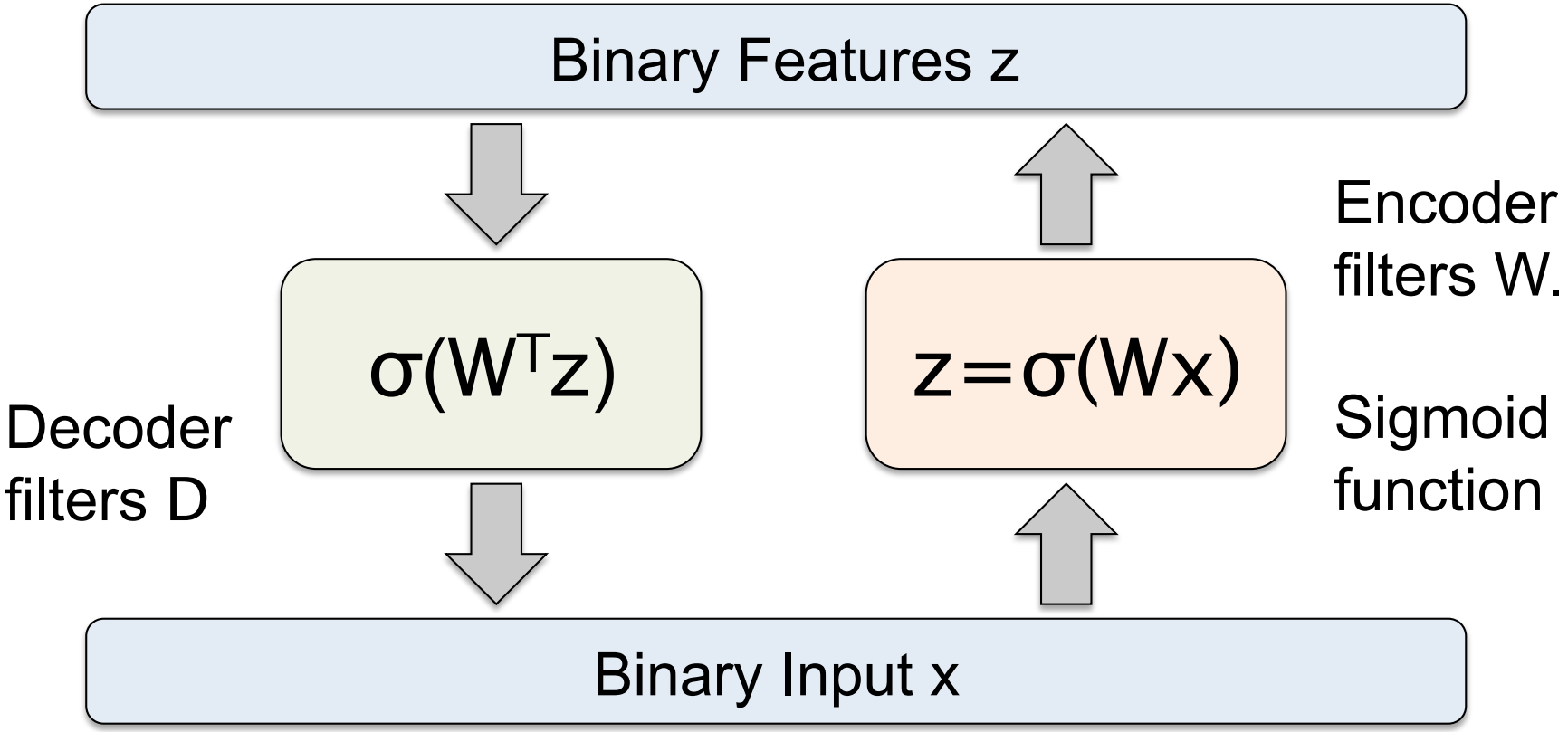


- If the hidden and output layers are linear, it will learn hidden units that are a linear function of the data and minimize the squared error.

- The K hidden units will span the same space as the first k principal components. The weight vectors may not be orthogonal.

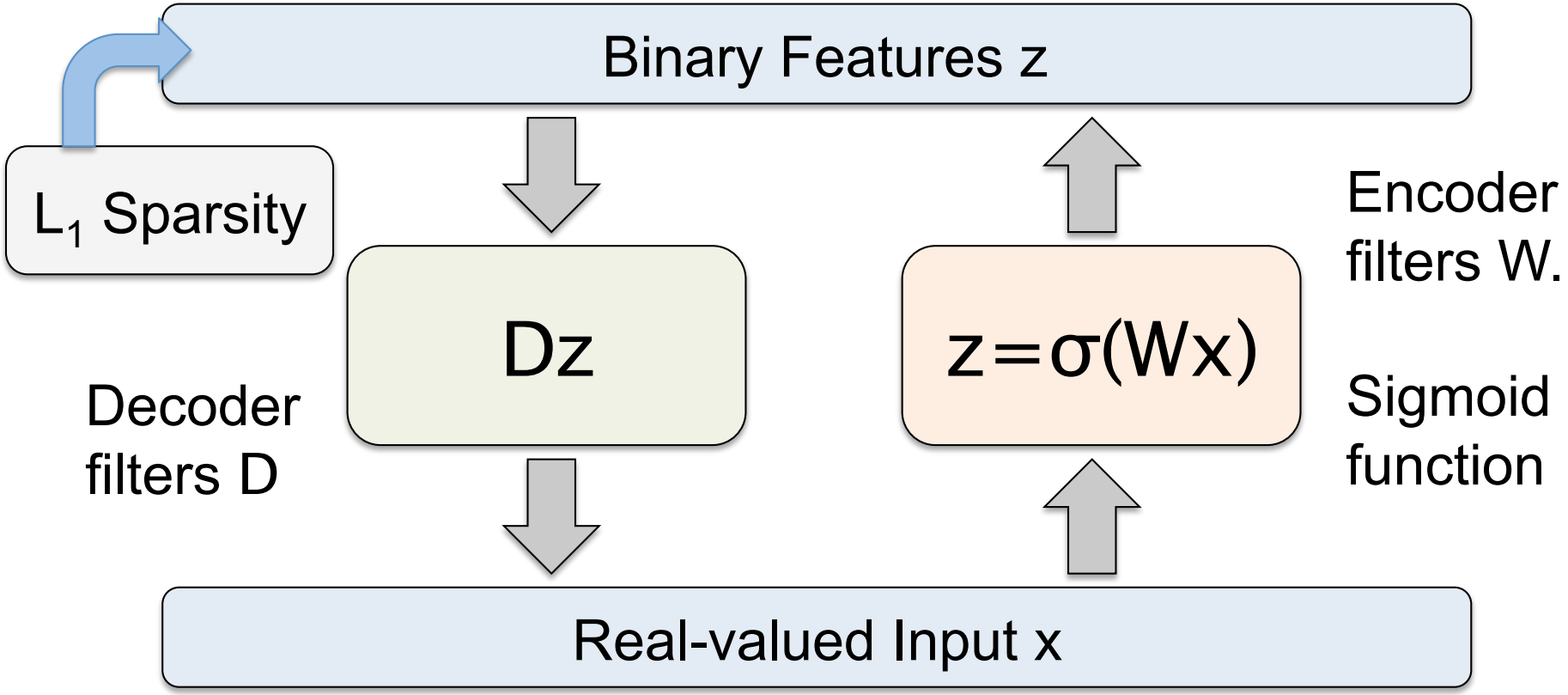
- With nonlinear hidden units, we have a nonlinear generalization of PCA.

Another Autoencoder Model



- Need additional constraints to avoid learning an identity.
- Relates to Restricted Boltzmann Machines (later).

Predictive Sparse Decomposition

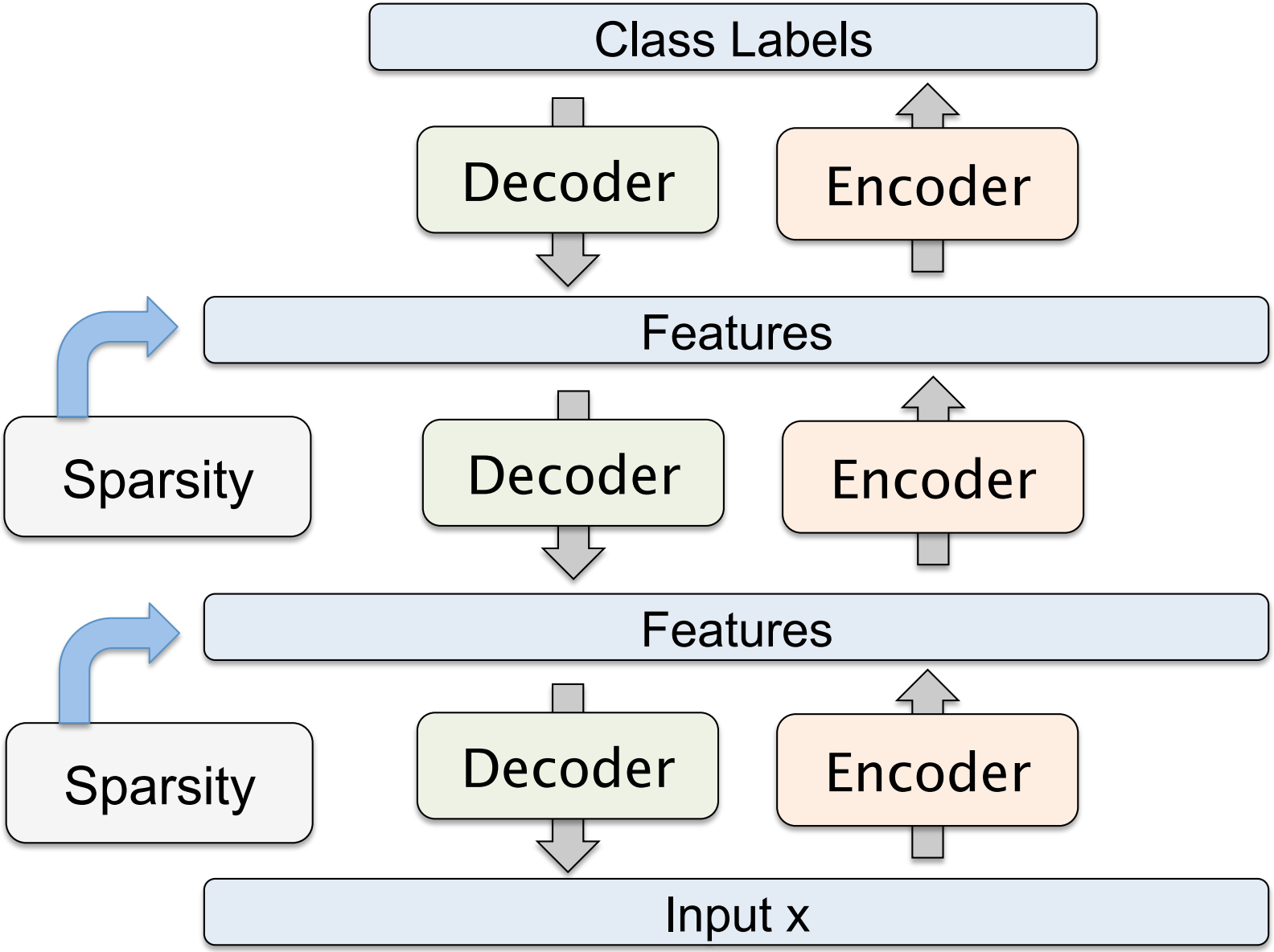


At training time

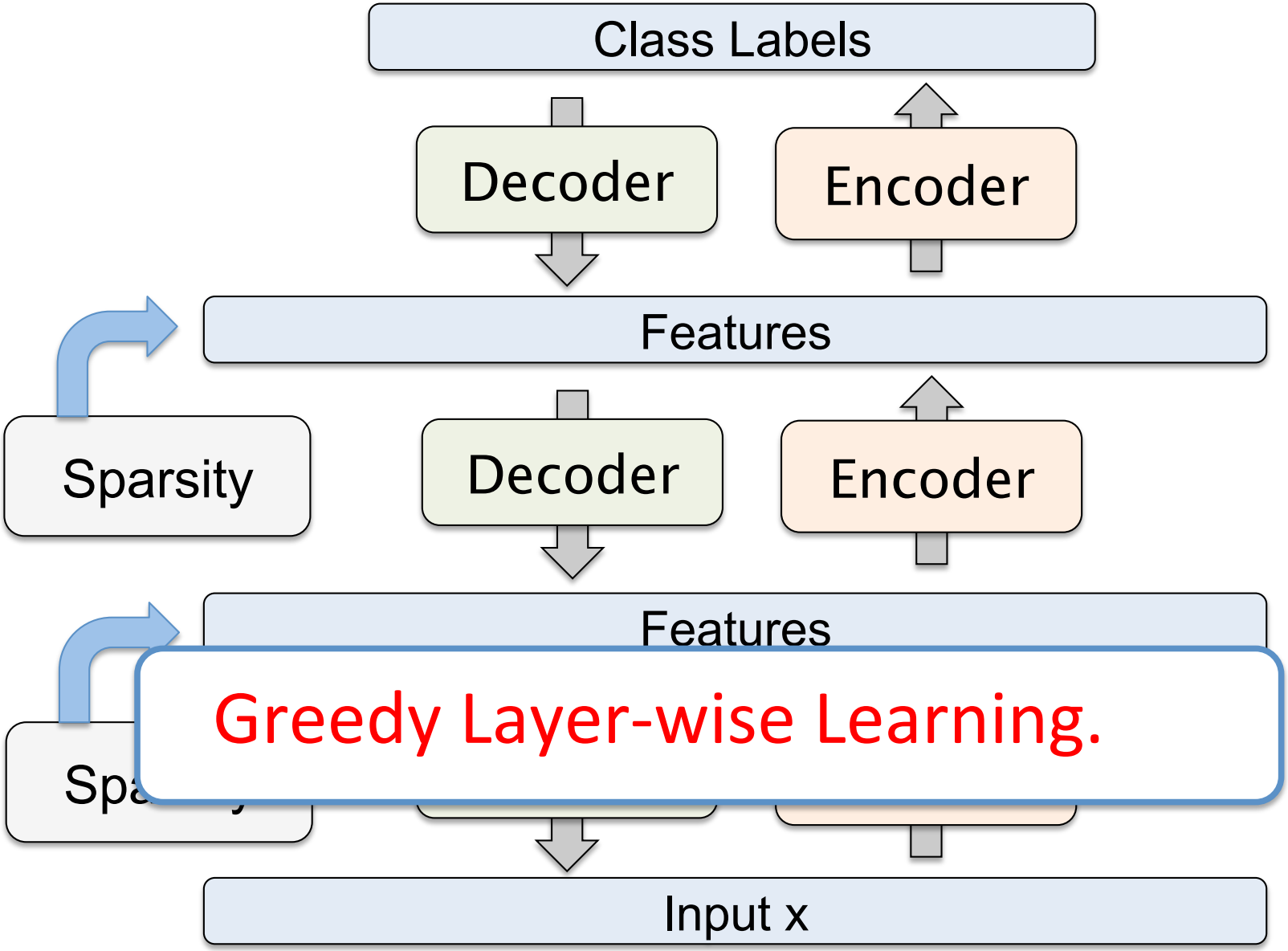
$$\min_{D,W,\mathbf{z}} \underbrace{||D\mathbf{z}-\mathbf{x}||_2^2+\lambda|\mathbf{z}|_1}_{\text{Decoder}} + \underbrace{||\sigma(W\mathbf{x})-\mathbf{z}||_2^2}_{\text{Encoder}}$$

Kavukcuoglu, Ranzato, Fergus, LeCun, 2009

Stacked Autoencoders

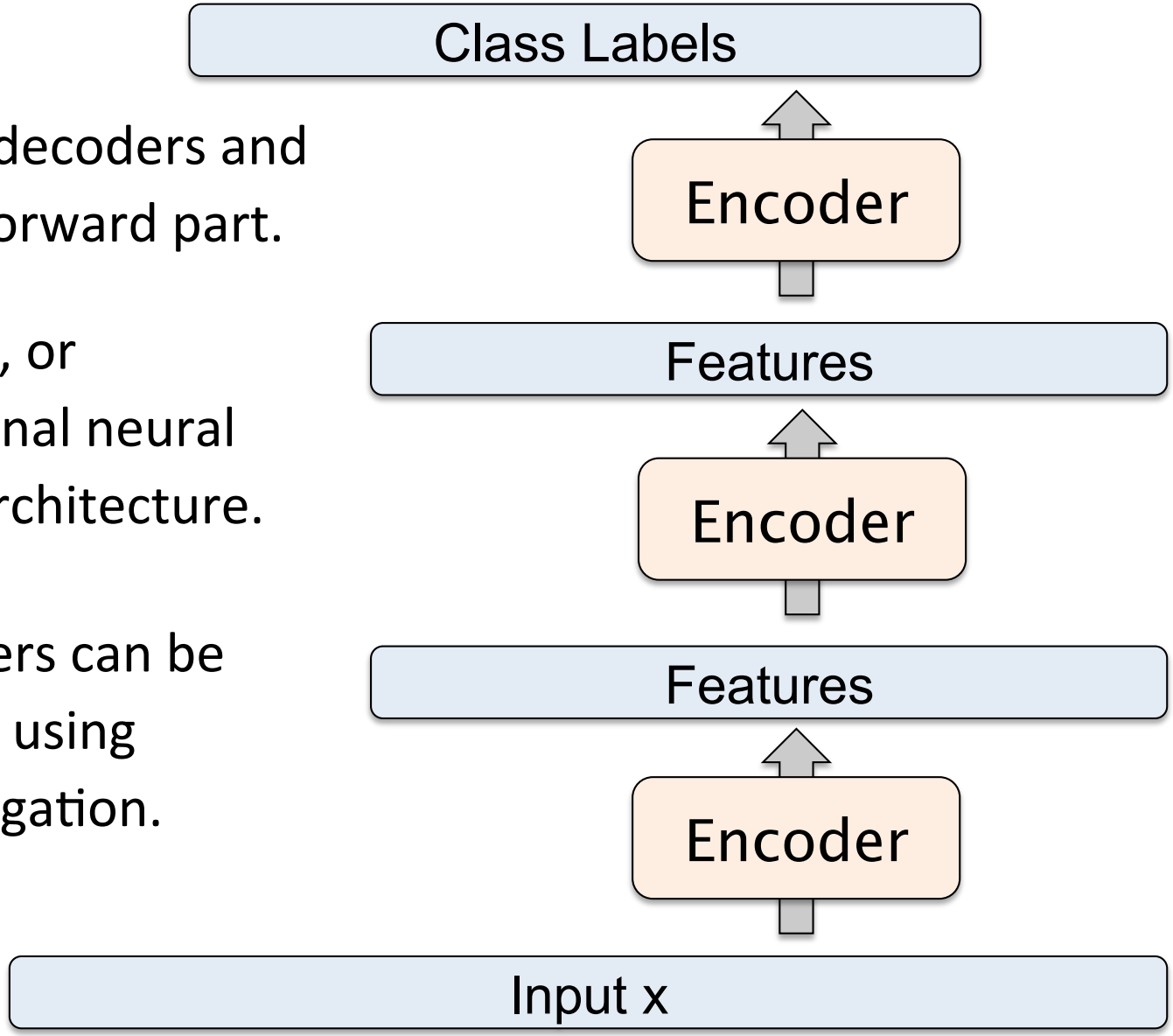


Stacked Autoencoders

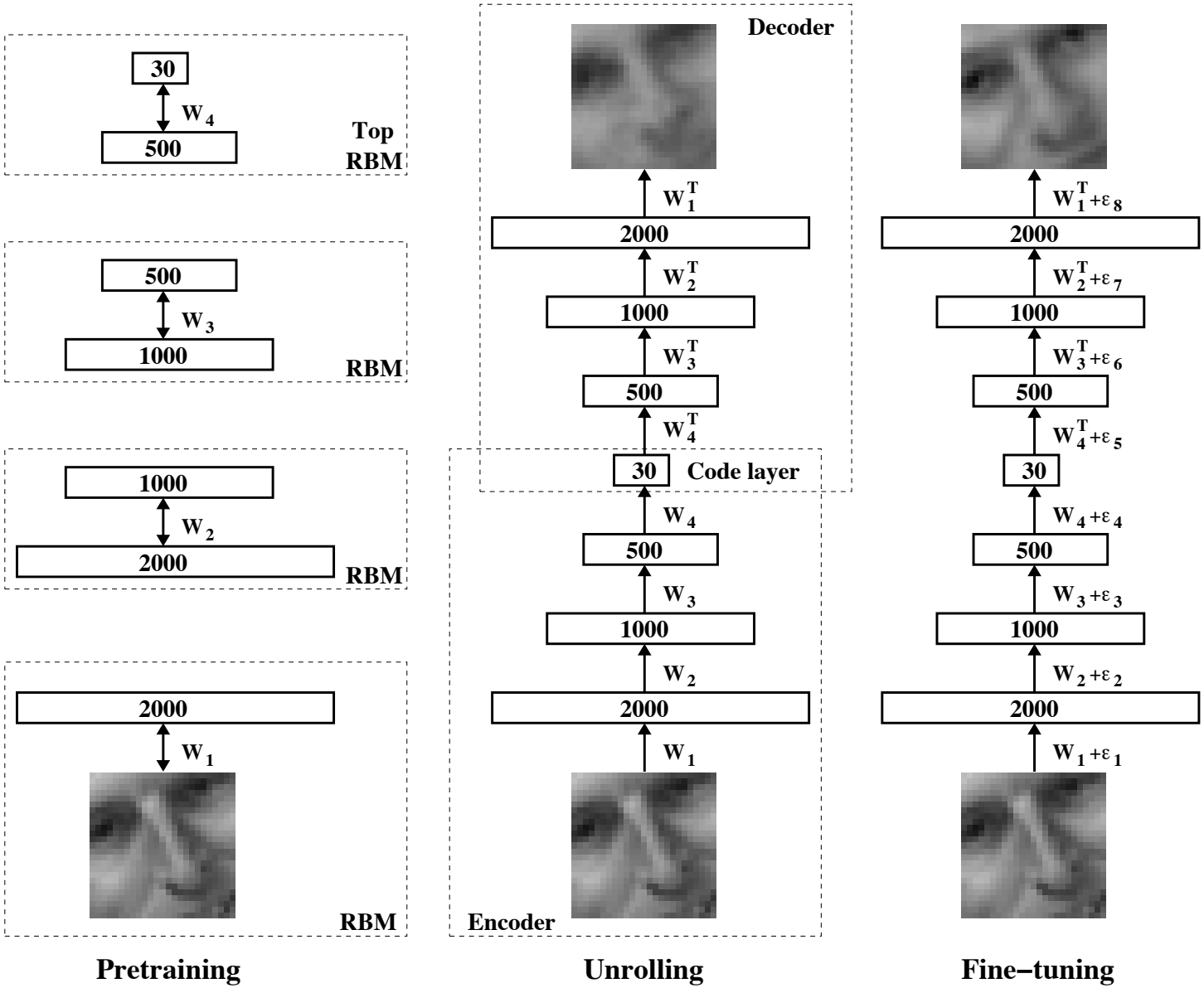


Stacked Autoencoders

- Remove decoders and use feed-forward part.
- Standard, or convolutional neural network architecture.
- Parameters can be fine-tuned using backpropagation.

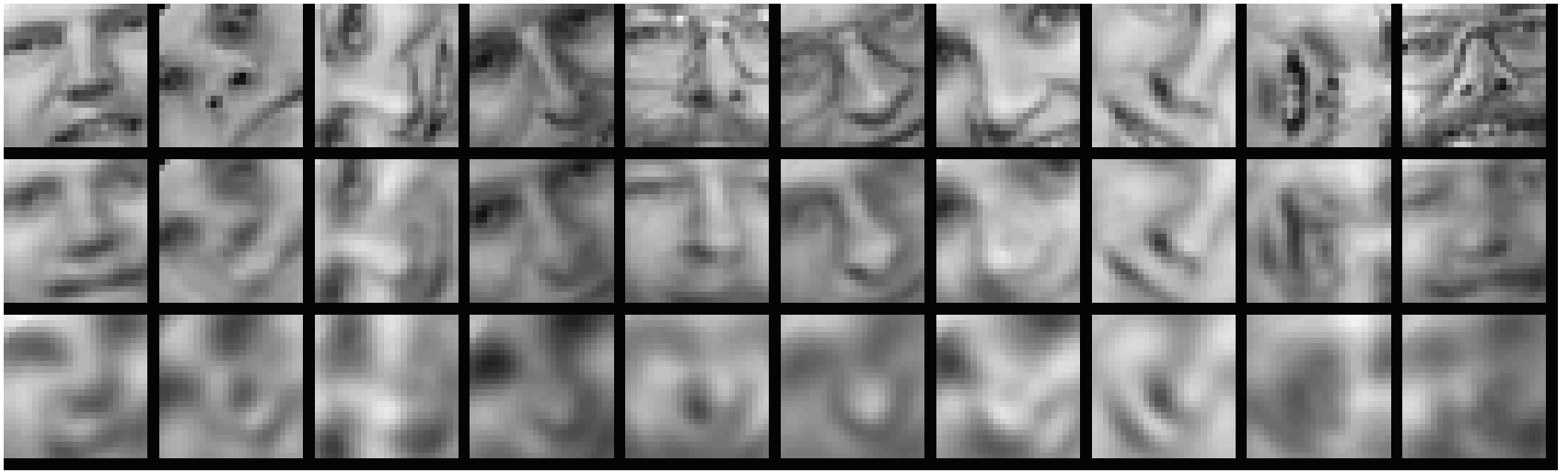


Deep Autoencoders



Deep Autoencoders

• 25x25 – 2000 – 1000 – 500 – 30 autoencoder to extract 30-D real-valued codes for Olivetti face patches.

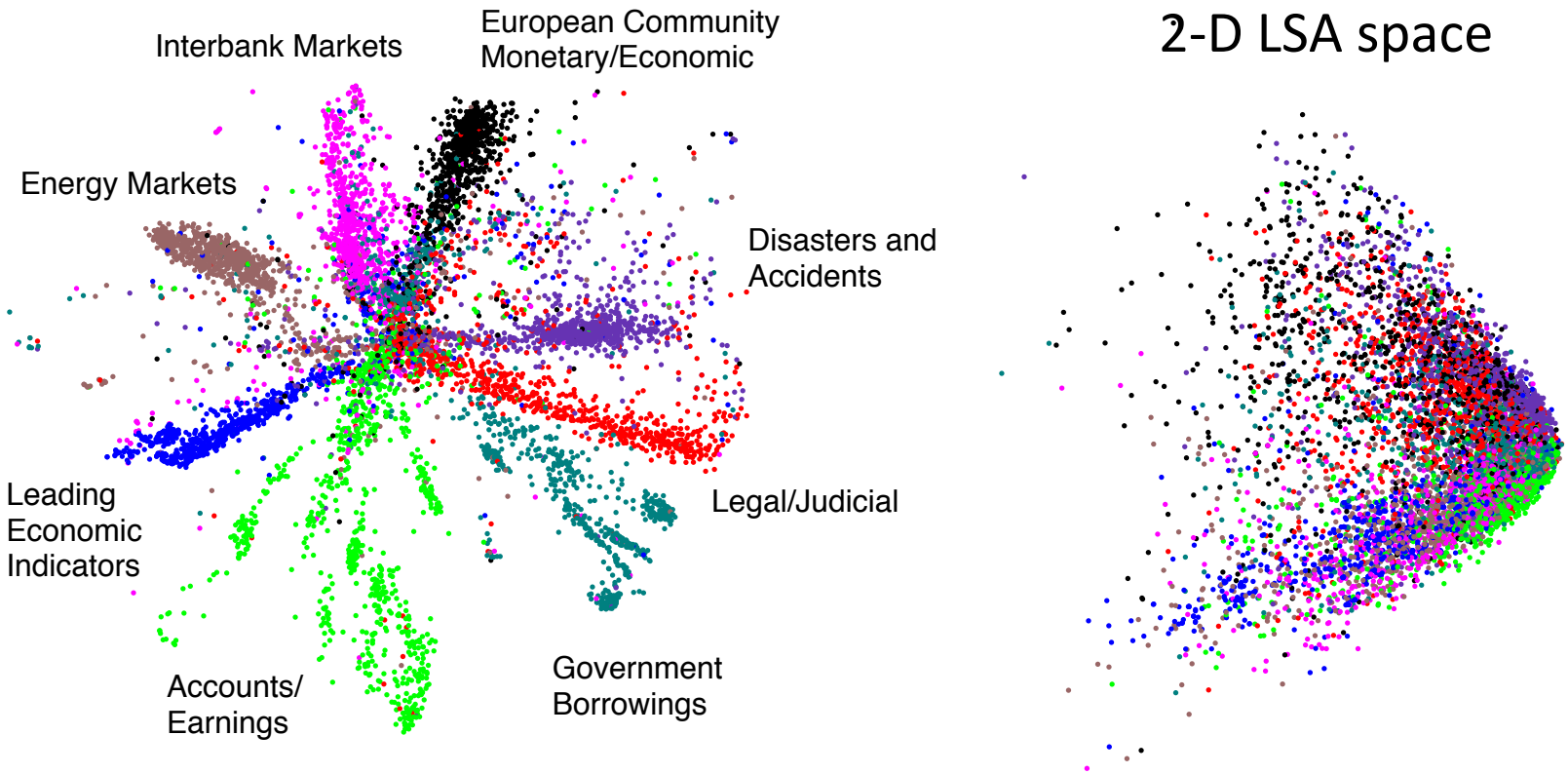


• **Top**: Random samples from the test dataset.

• **Middle**: Reconstructions by the 30-dimensional deep autoencoder.

• **Bottom**: Reconstructions by the 30-dimentinoal PCA.

Information Retrieval



- The Reuters Corpus Volume II contains 804,414 newswire stories (randomly split into **402,207 training** and **402,207 test).**
- "Bag-of-words" representation: each article is represented as a vector containing the counts of the most frequently used 2000 words.

(Hinton and Salakhutdinov, Science 2006)

Tutorial Roadmap

- Basic Building Blocks:
  - Sparse Coding
  - Autoencoders
- Deep Generative Models
  - Restricted Boltzmann Machines
  - Deep Boltzmann Machines
  - Helmholtz Machines / Variational Autoencoders
- Generative Adversarial Networks

Fully Observed Models

- Explicitly model conditional probabilities:

$$p_{\text{model}}(\boldsymbol{x}) = p_{\text{model}}(x_1) \prod_{i=2}^{n} p_{\text{model}}(x_i \mid x_1, \ldots, x_{i-1})$$

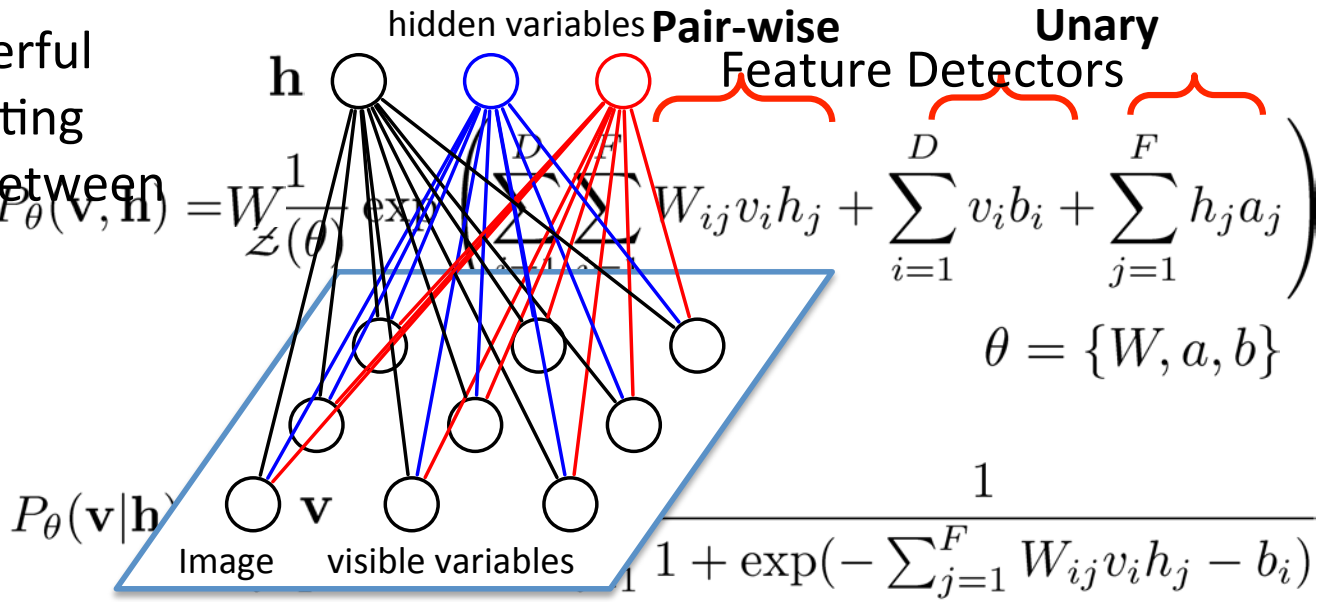
Each conditional can be a complicated neural network

- A number of successful models, including
  - NADE, RNADE (Larochelle, et.al. 20011)
  - Pixel CNN (van den Ord et. al. 2016)
  - Pixel RNN (van den Ord et. al. 2016)

Pixel CNN

Restricted Boltzmann Machines

Graphical Models: Powerful framework for representing dependency structure between random variables.



RBM is a Markov Random Field with:

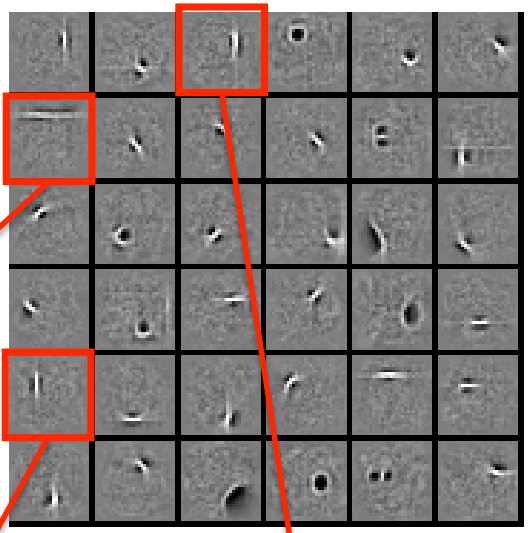
- Stochastic binary visible variables $\mathbf{v} \in \{0,1\}^D$.
- Stochastic binary hidden variables $\mathbf{h} \in \{0,1\}^F$.
- Bipartite connections.

Markov random fields, Boltzmann machines, log-linear models.

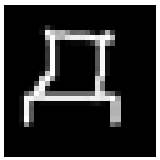
Learning Features

Observed Data
Subset of 25,000 characters

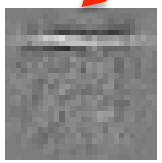
Learned W: "edges"
Subset of 1000 features



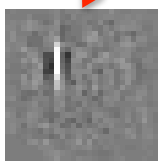
New Image:



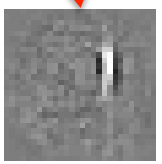
$$= \sigma\left(0.99 \times \right.$$



$$+ \quad 0.97 \times$$



$$+ \quad 0.82 \times$$



$$\left. \cdots \right)$$

$p(h_7 = 1|v)$

$p(h_{29} = 1|v)$

Sparse representations

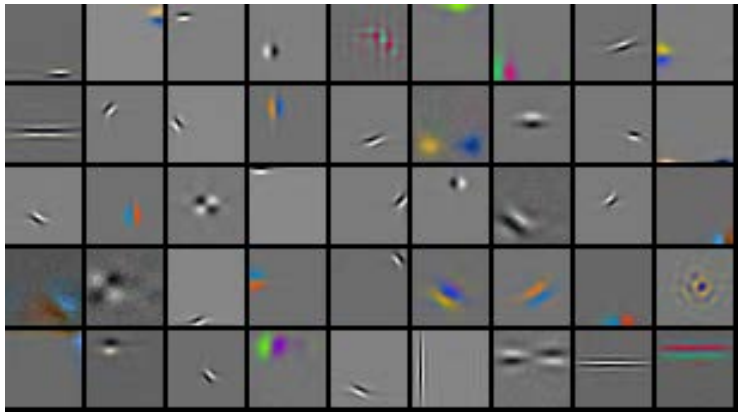
$$\sigma(x) = \frac{1}{1+\exp(-x)}$$

Logistic Function: Suitable for modeling binary images

RBMs for Real-valued & Count Data

4 million **unlabelled** images

Learned features (out of 10,000)



Reuters dataset:
804,414 **unlabeled**
newswire stories
Bag-of-Words

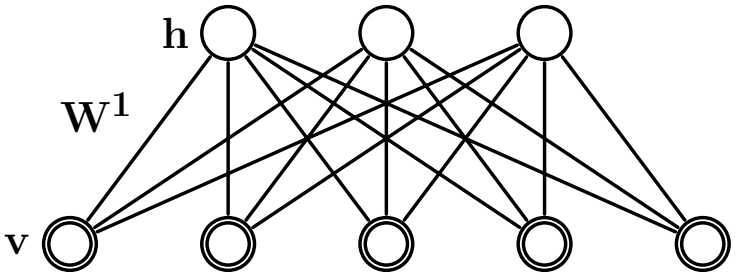
Learned features: ``topics''

russian	clinton	computer	trade	stock
russia	house	system	country	wall
moscow	president	product	import	street
yeltsin	bill	software	world	point
soviet	congress	develop	economy	dow

Collaborative Filtering

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{ijk} W_{ij}^k v_i^k h_j + \sum_{ik} b_i^k v_i^k + \sum_j a_j h_j \right)$$

Binary hidden: user preferences



Multinomial visible: user ratings

Netflix dataset:
480,189 users
17,770 movies
Over 100 million ratings

Learned features: ``genre''

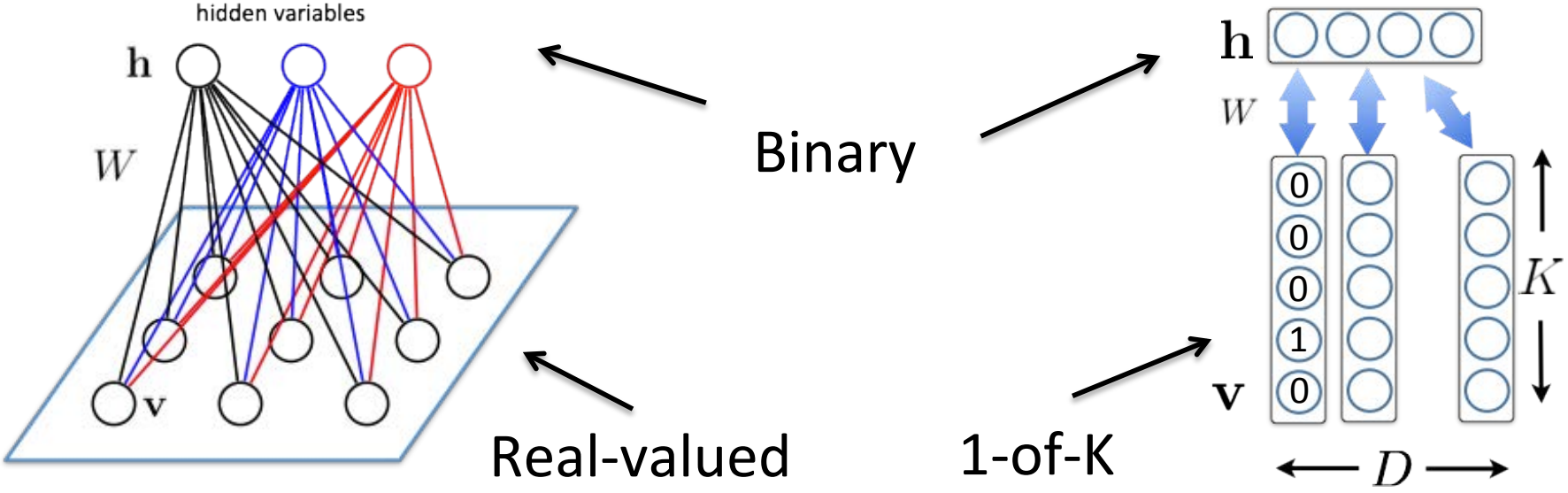
Fahrenheit 9/11	Independence Day
Bowling for Columbine	The Day After Tomorrow
The People vs. Larry Flynt	Con Air
Canadian Bacon	Men in Black II
La Dolce Vita	Men in Black
Friday the 13th	Scary Movie
The Texas Chainsaw Massacre	Naked Gun
Children of the Corn	Hot Shots!
Child's Play	American Pie
The Return of Michael Myers	Police Academy

State-of-the-art performance on the Netflix dataset.

(Salakhutdinov, Mnih, Hinton, ICML 2007)

Different Data Modalities

• Binary/Gaussian/Softmax RBMs: All have binary hidden variables but use them to model different kinds of data.



• It is easy to infer the states of the hidden variables:

$$P_\theta(\mathbf{h}|\mathbf{v}) = \prod_{j=1}^{F} P_\theta(h_j|\mathbf{v}) = \prod_{j=1}^{F} \frac{1}{1+\exp(-a_j - \sum_{i=1}^{D} W_{ij} v_i)}$$

Product of Experts

The joint distribution is given by:

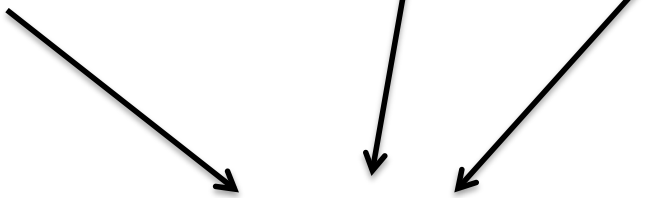
$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij} W_{ij} v_i h_j + \sum_i b_i v_i + \sum_j a_j h_j\Big)$$

Marginalizing over hidden variables:

Product of Experts

$$P_\theta(\mathbf{v}) = \sum_{\mathbf{h}} P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \prod_i \exp(b_i v_i) \prod_j \Big(1 + \exp(a_j + \sum_i W_{ij} v_i)\Big)$$

government authority power empire federation	clinton house president bill congress	bribery corruption dishonesty corrupt fraud	mafia business gang mob insider	stock wall street point dow	…



Silvio Berlusconi

Topics “government”, ”corruption” and ”mafia” can combine to give very high probability to a word “Silvio Berlusconi”.

Product of Experts

The joint distribution is given by:

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij} W_{ij} v_i h_j + \sum_i b_i v_i + \sum_j a_j h_j\Big)$$

Marginalizing o

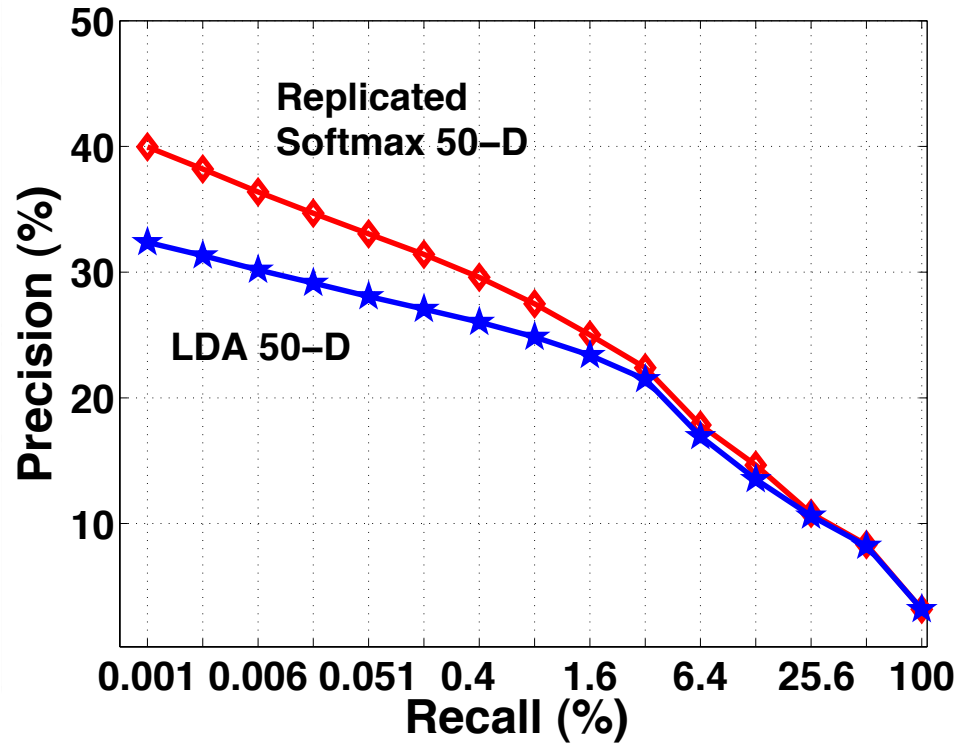
$$P_\theta(\mathbf{v}) = \sum_{\mathbf{h}}$$

duct of Experts

$$W_{ij} v_i)\Big)$$

government
authority
power
empire
federation

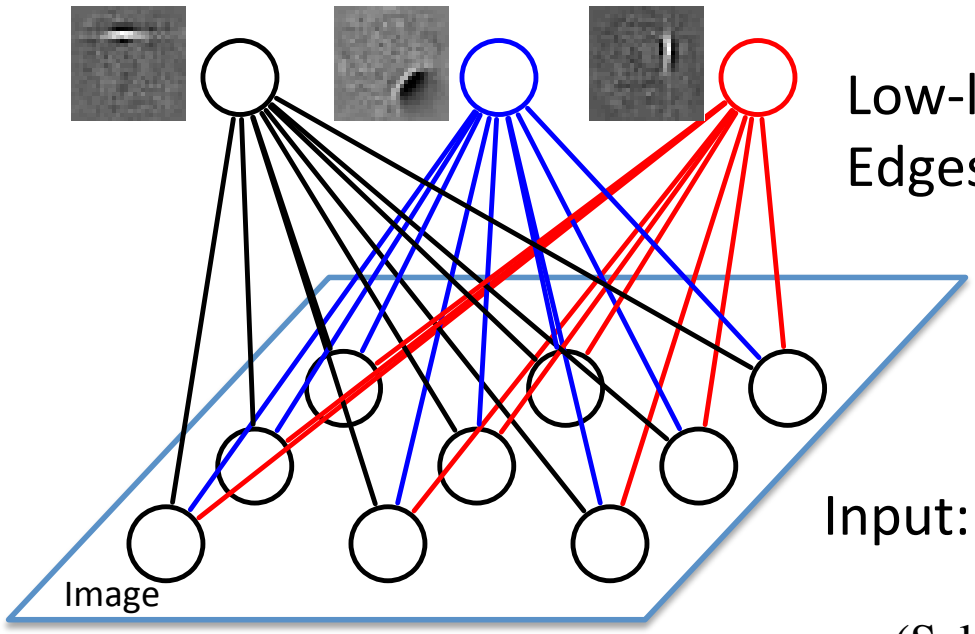
clint
hou
pres
bill
cong



, "corruption"
bine to give very
word "Silvio

Berlusconi".

Deep Boltzmann Machines



Low-level features:
Edges

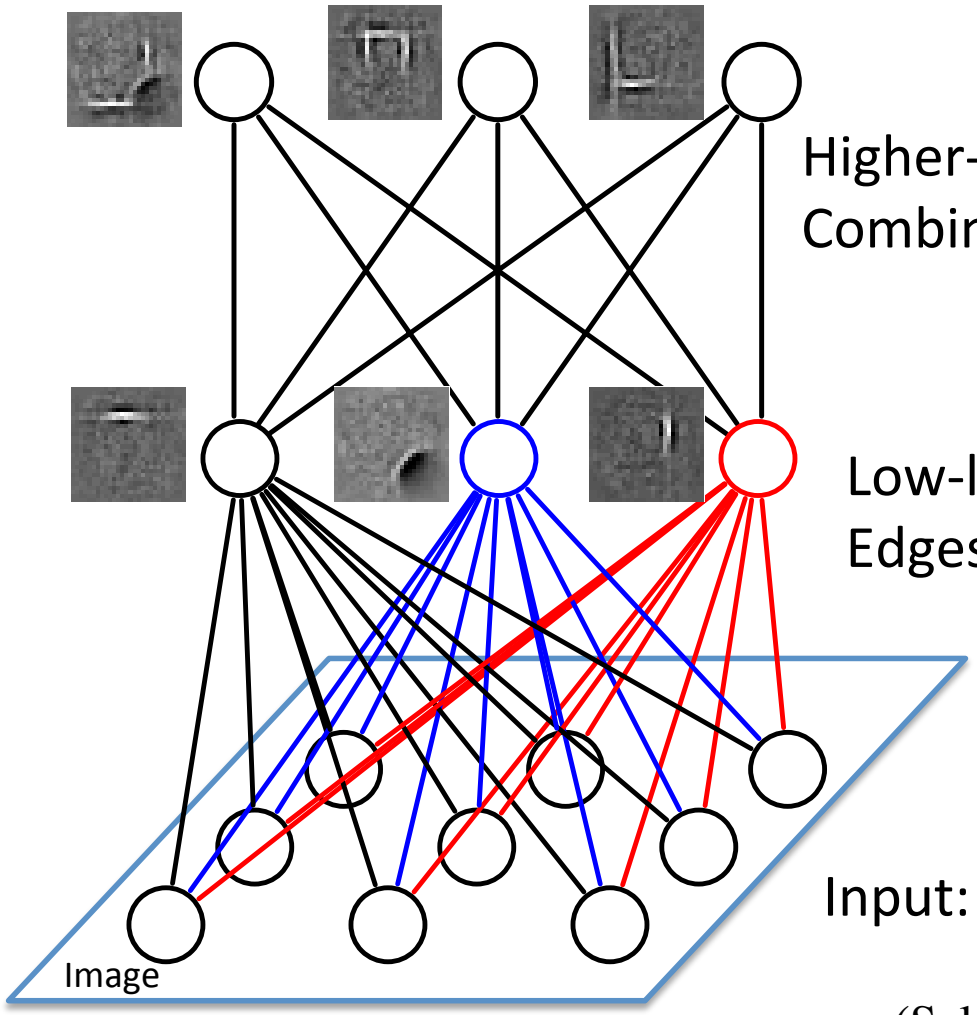
Built from **unlabeled** inputs.

Input: Pixels

(Salakhutdinov 2008, Salakhutdinov & Hinton 2012)

Deep Boltzmann Machines

Learn simpler representations,
then compose more complex ones



Higher-level features:
Combination of edges

Low-level features:
Edges

Input: Pixels

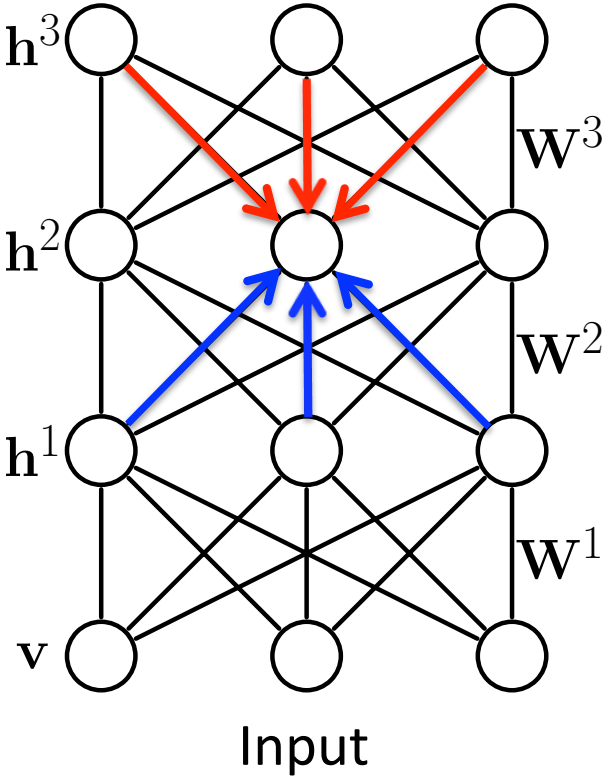
Built from **unlabeled** inputs.

(Salakhutdinov 2008, Salakhutdinov & Hinton 2009)

Model Formulation

$$P_\theta(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left[\mathbf{v}^\top W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)\top} W^{(3)} \mathbf{h}^{(3)}\right]$$

Same as RBMs



$\theta = \{W^1, W^2, W^3\}$ model parameters

- Dependencies between hidden variables.
- All connections are undirected.
- Bottom-up and Top-down:

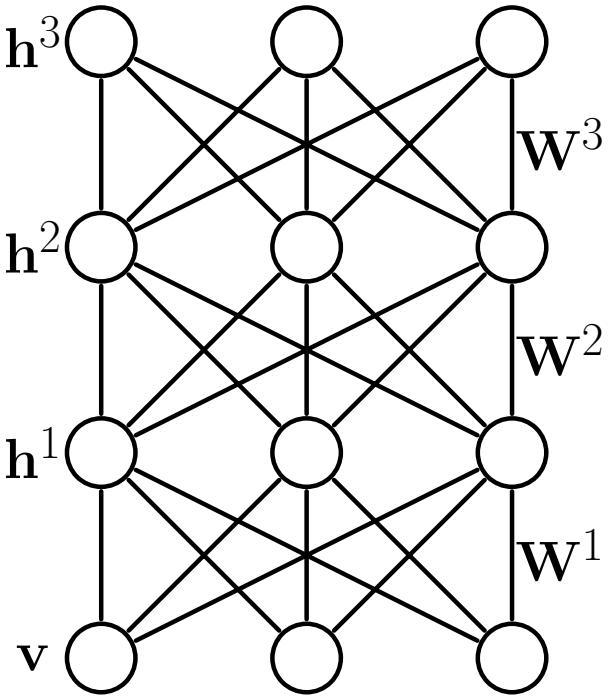
$$P(h_j^2 = 1 | \mathbf{h}^1, \mathbf{h}^3) = \sigma\left(\sum_k W_{kj}^3 h_k^3 + \sum_m W_{mj}^2 h_m^1\right)$$

Top-down Bottom-up

- Hidden variables are dependent even when **conditioned on the input**.

Approximate Learning

$$P_\theta(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left[\mathbf{v}^\top W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)\top} W^{(3)} \mathbf{h}^{(3)}\right]$$



(Approximate) Maximum Likelihood:

$$\frac{\partial \log P_\theta(\mathbf{v})}{\partial W^1} = \mathbb{E}_{P_{data}}[\mathbf{v}\mathbf{h^1}^\top] - \mathbb{E}_{P_\theta}[\mathbf{v}\mathbf{h^1}^\top]$$

- Both expectations are intractable!

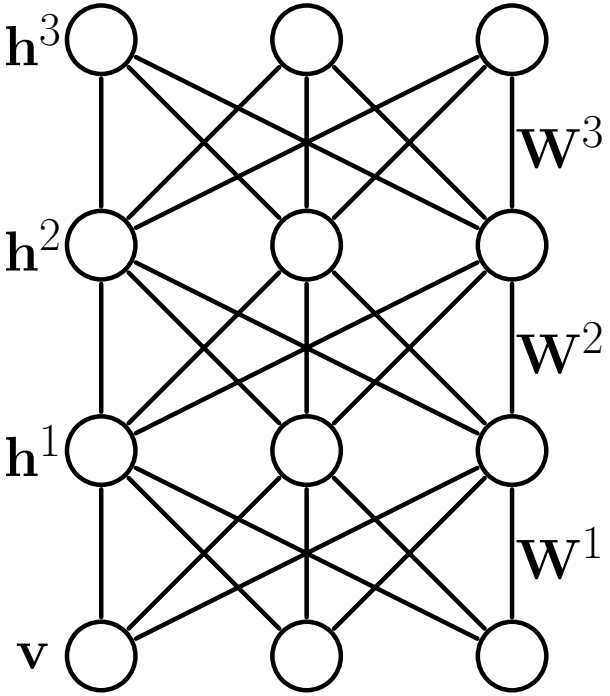
$$P_{data}(\mathbf{v}, \mathbf{h^1}) = P_\theta(\mathbf{h^1}|\mathbf{v}) P_{data}(\mathbf{v})$$

$$P_{data}(\mathbf{v}) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v_n})$$

Not factorial any more!

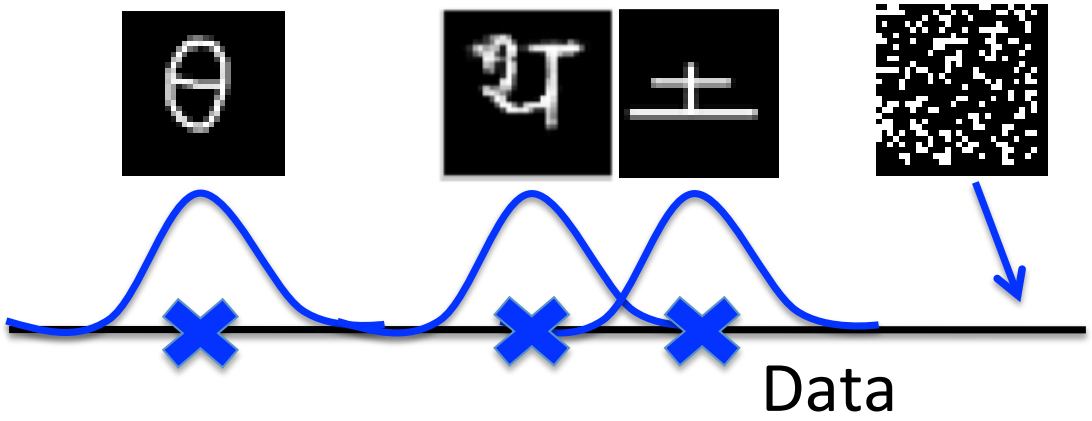
Approximate Learning

$$P_\theta(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left[\mathbf{v}^\top W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)\top} W^{(3)} \mathbf{h}^{(3)}\right]$$



(Approximate) Maximum Likelihood:

$$\frac{\partial \log P_\theta(\mathbf{v})}{\partial W^1} = \mathbb{E}_{P_{data}}[\mathbf{v}\mathbf{h^1}^\top] - \mathbb{E}_{P_\theta}[\mathbf{v}\mathbf{h^1}^\top]$$



$$P_{data}(\mathbf{v}, \mathbf{h^1}) = P_\theta(\mathbf{h^1}|\mathbf{v}) P_{data}(\mathbf{v})$$

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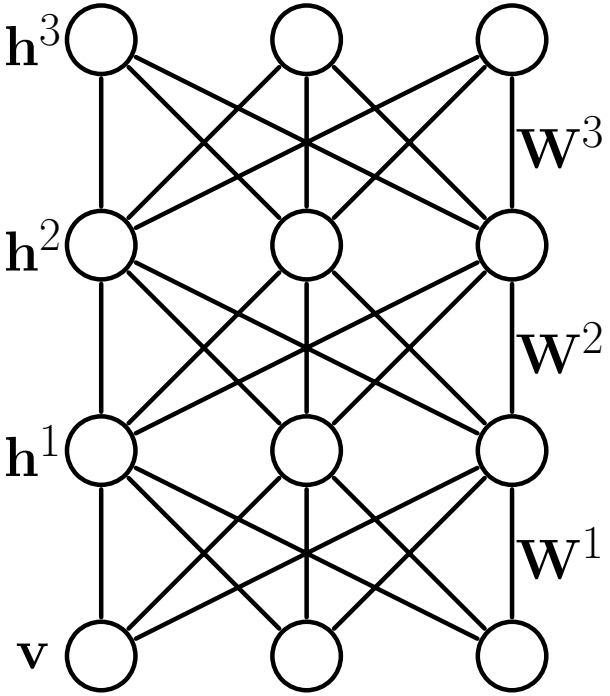
Not factorial any more!

Approximate Learning

$$P_\theta(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left[\mathbf{v}^\top W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)\top} W^{(3)} \mathbf{h}^{(3)}\right]$$



(Approximate) Maximum Likelihood:

$$\frac{\partial \log P_\theta(\mathbf{v})}{\partial W^1} = \mathbb{E}_{P_{data}}[\mathbf{v}\mathbf{h^1}^\top] - \mathbb{E}_{P_\theta}[\mathbf{v}\mathbf{h^1}^\top]$$

Variational Inference

Stochastic Approximation (MCMC-based)

$$P_{data}(\mathbf{v}, \mathbf{h^1}) = P_\theta(\mathbf{h^1}|\mathbf{v}) P_{data}(\mathbf{v})$$

$$P_{data}(\mathbf{v}) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{v} - \mathbf{v_n})$$

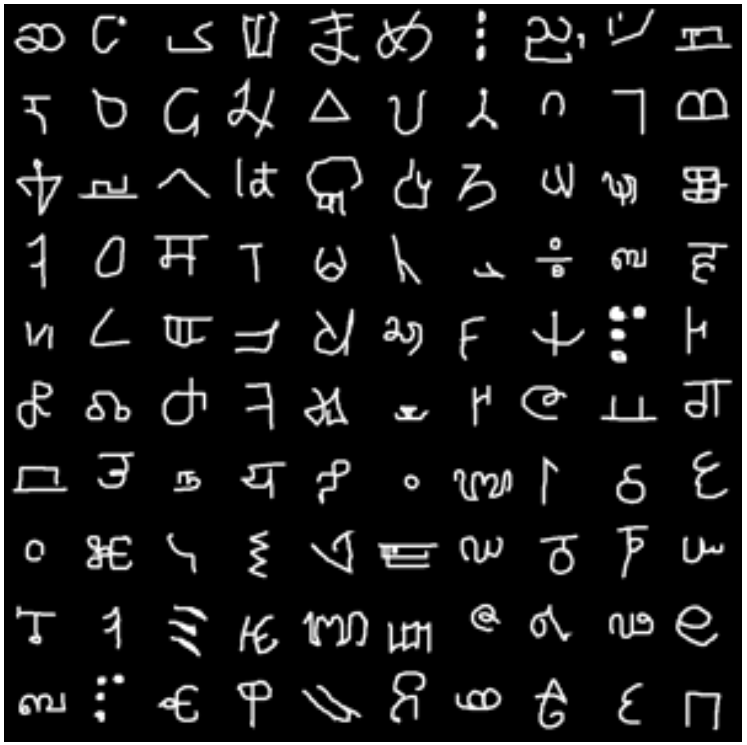
Not factorial any more!

Good Generative Model?

Handwritten Characters

Good Generative Model?

Handwritten Characters



Good Generative Model?

Handwritten Characters

Simulated

Real Data

Good Generative Model?

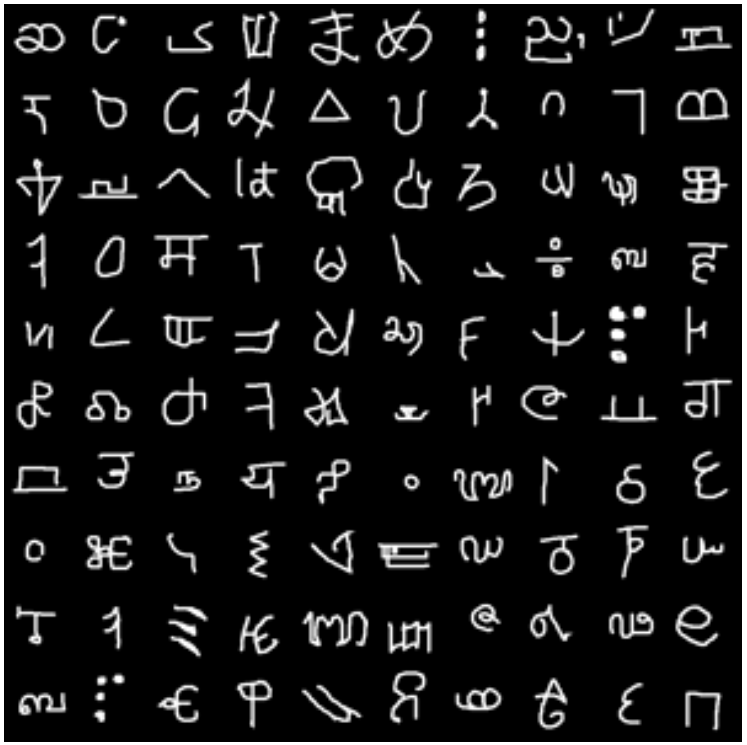
Handwritten Characters

Real Data

Simulated

Good Generative Model?

Handwritten Characters



Handwriting Recognition

MNIST Dataset
60,000 examples of 10 digits

Learning Algorithm	Error
Logistic regression	12.0%
K-NN	3.09%
Neural Net (Platt 2005)	1.53%
SVM (Decoste et.al. 2002)	1.40%
Deep Autoencoder (Bengio et. al. 2007)	1.40%
Deep Belief Net (Hinton et. al. 2006)	1.20%
DBM	**0.95%**

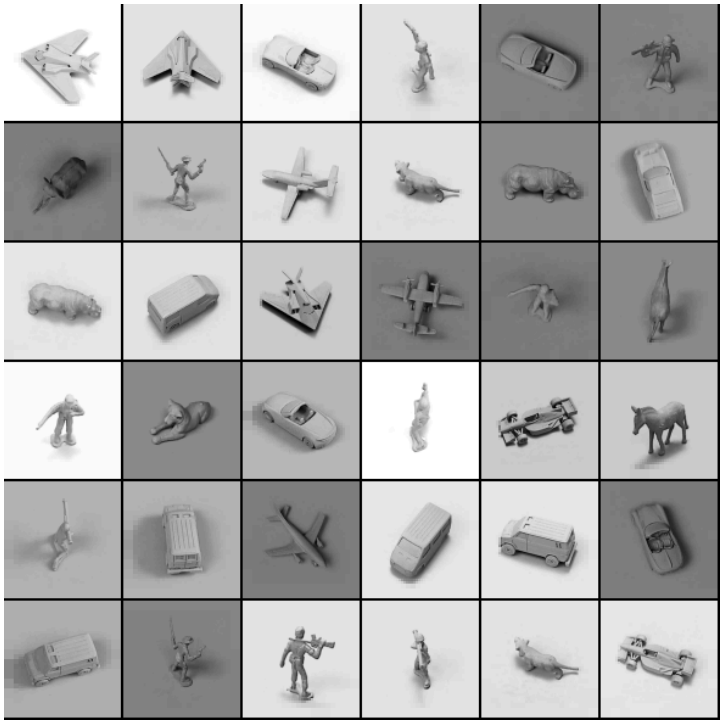
Optical Character Recognition
42,152 examples of 26 English letters

Learning Algorithm	Error
Logistic regression	22.14%
K-NN	18.92%
Neural Net	14.62%
SVM (Larochelle et.al. 2009)	9.70%
Deep Autoencoder (Bengio et. al. 2007)	10.05%
Deep Belief Net (Larochelle et. al. 2009)	9.68%
DBM	**8.40%**

Permutation-invariant version.

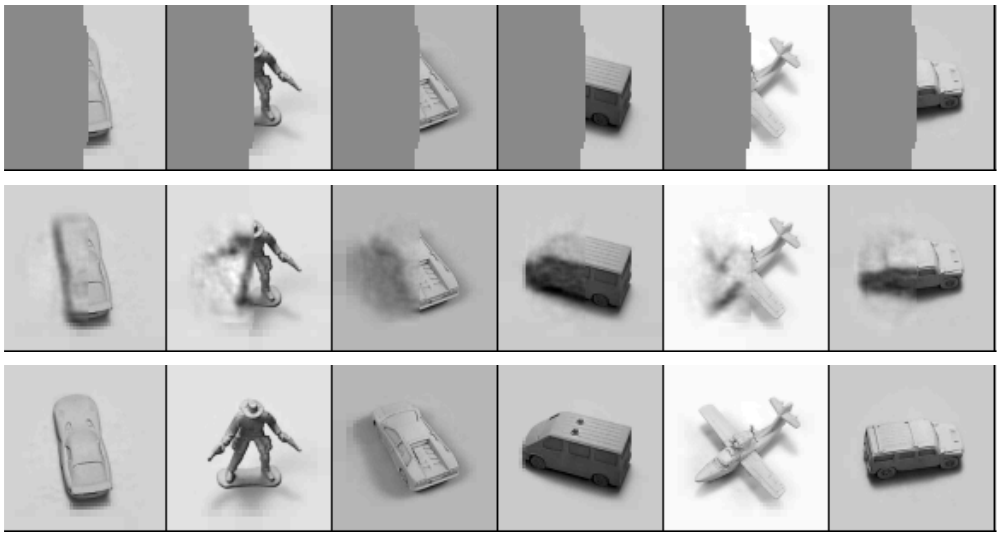
3-D object Recognition

NORB Dataset: 24,000 examples



Learning Algorithm	Error
Logistic regression	22.5%
K-NN (LeCun 2004)	18.92%
SVM (Bengio & LeCun 2007)	11.6%
Deep Belief Net (Nair & Hinton 2009)	9.0%
DBM	**7.2%**

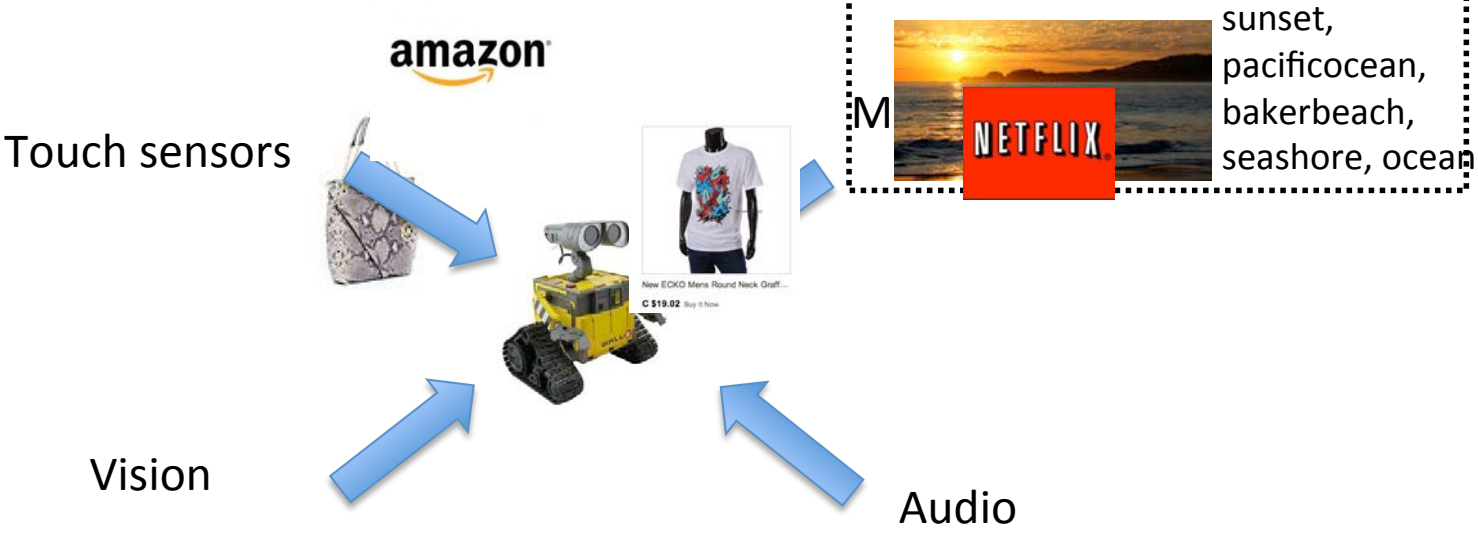
Pattern Completion



Data – Collection of Modalities

- Multimedia content on the web - image + text + audio.
- Product recommendation systems.
- Robotics application

car, automobile



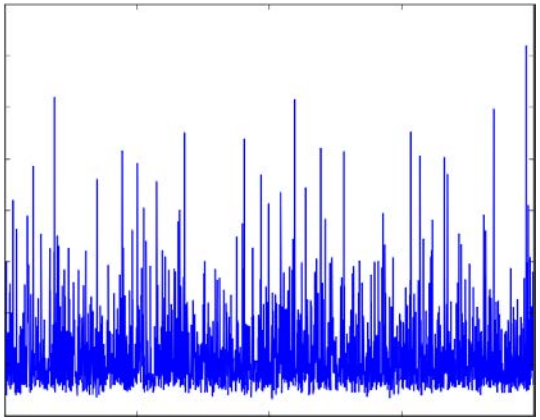
Challenges - I

Image

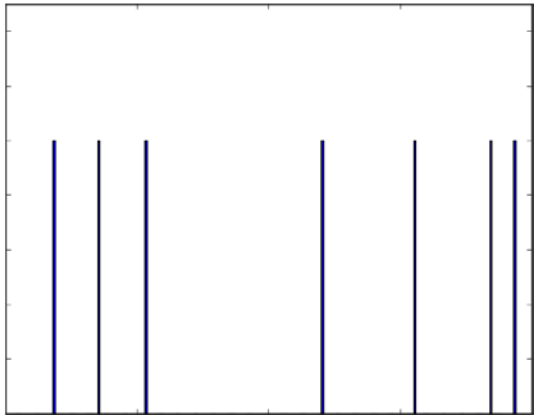
Text

sunset, pacific ocean, baker beach, seashore, ocean

Dense



Sparse



Very different input representations

- Images – real-valued, dense
- Text – discrete, sparse

Difficult to learn cross-modal features from low-level representations.

Challenges - II

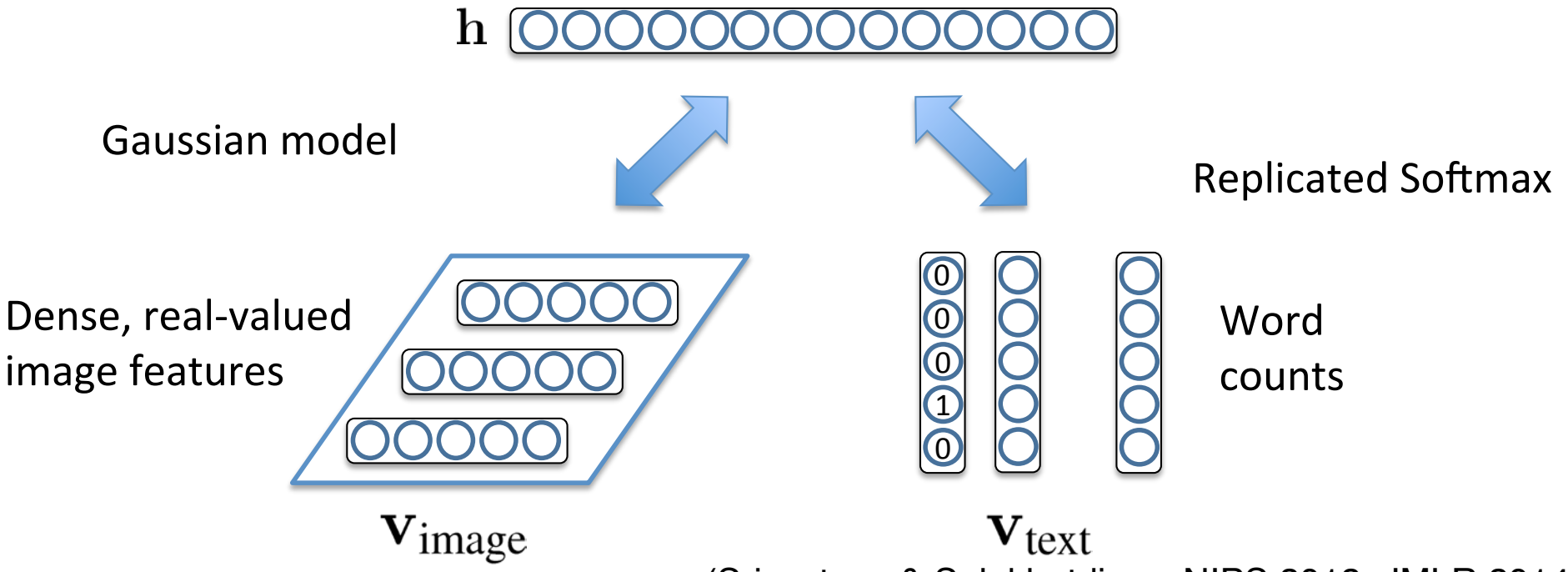
Image	Text
	pentax, k10d, pentaxda50200, kangarooisland, sa, australiansealion
	mickikrimmel, mickipedia, headshot
	< no text>
	unseulpixel, naturey

Noisy and missing data

Challenges - II

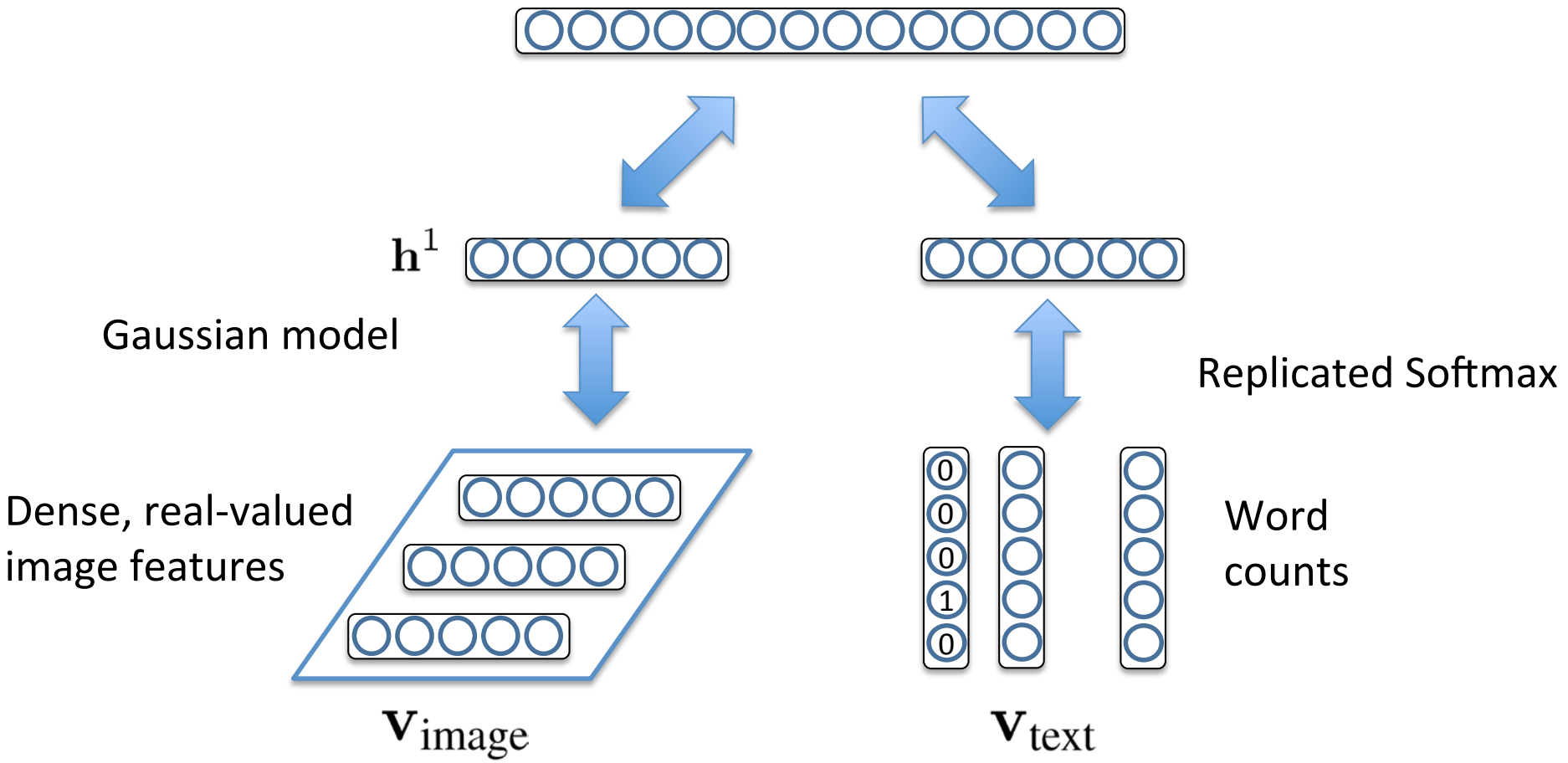
Image	Text	Text generated by the model
	pentax, k10d, pentaxda50200, kangarooisland, sa, australiansealion	beach, sea, surf, strand, shore, wave, seascape, sand, ocean, waves
	mickikrimmel, mickipedia, headshot	portrait, girl, woman, lady, blonde, pretty, gorgeous, expression, model
	< no text>	night, notte, traffic, light, lights, parking, darkness, lowlight, nacht, glow
	unseulpixel, naturey	fall, autumn, trees, leaves, foliage, forest, woods, branches, path

Multimodal DBM



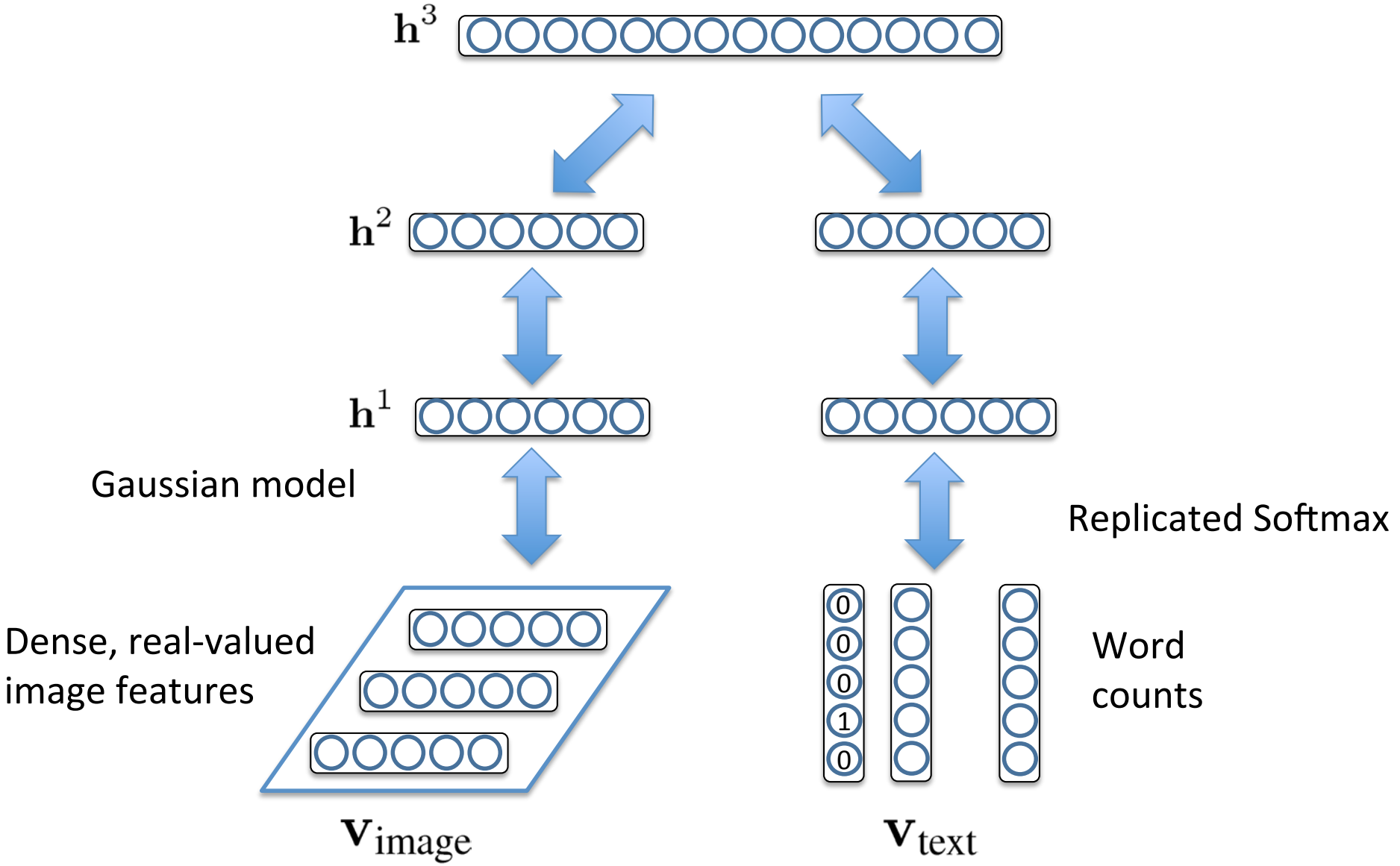
(Srivastava & Salakhutdinov, NIPS 2012, JMLR 2014)

Multimodal DBM



(Srivastava & Salakhutdinov, NIPS 2012, JMLR 2014)

Multimodal DBM



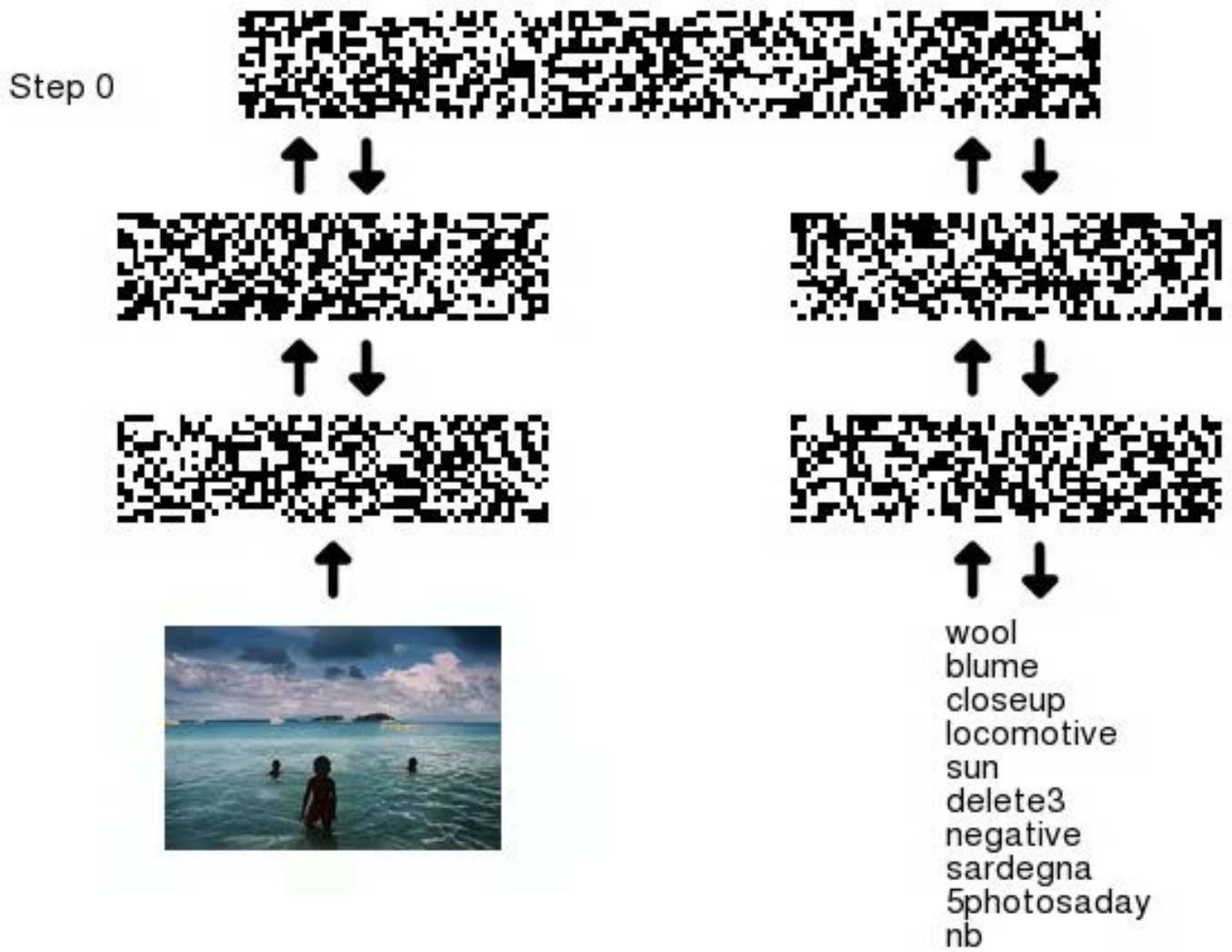
(Srivastava & Salakhutdinov, NIPS 2012, JMLR 2014)

Text Generated from Images

Given	Generated
	dog, cat, pet, kitten, puppy, ginger, tongue, kitty, dogs, furry
	sea, france, boat, mer, beach, river, bretagne, plage, brittany
	portrait, child, kid, ritratto, kids, children, boy, cute, boys, italy

Given	Generated
	insect, butterfly, insects, bug, butterflies, lepidoptera
	graffiti, streetart, stencil, sticker, urbanart, graff, sanfrancisco
	canada, nature, sunrise, ontario, fog, mist, bc, morning

Generating Text from Images



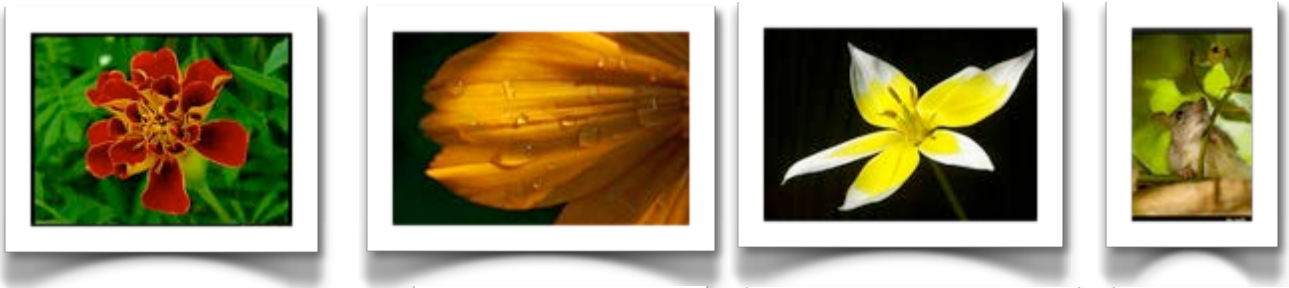
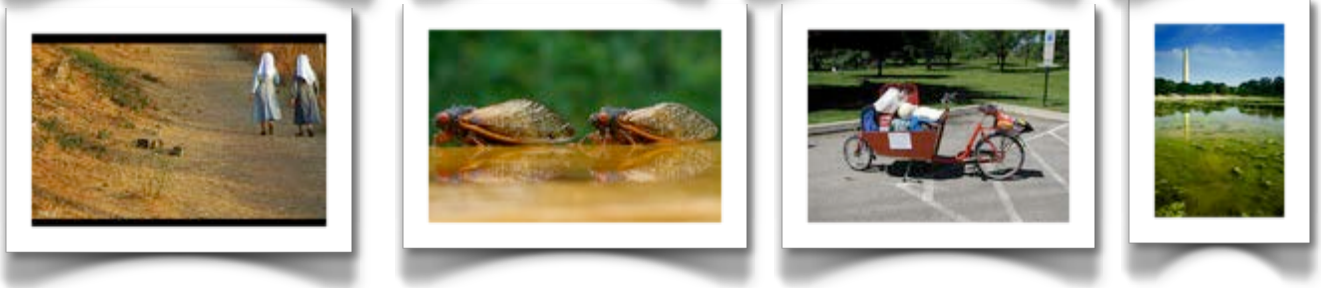
Samples drawn after every 50 steps of Gibbs updates

Sample at step 0
wool
blume
closeup
locomotive
sun
delete3
negative
sardegna
5photosaday
nb

Text Generated from Images

Given	Generated
	portrait, women, army, soldier, mother, postcard, soldiers
	obama, barackobama, election, politics, president, hope, change, sanfrancisco, convention, rally
	water, glass, beer, bottle, drink, wine, bubbles, splash, drops, drop

Images from Text

Given	Retrieved
water, red, sunset	
nature, flower, red, green	
blue, green, yellow, colors	
chocolate, cake	

MIR-Flickr Dataset

- 1 million images along with user-assigned tags.

sculpture, beauty, stone

d80

nikon, abigfave, goldstaraward, d80, nikond80

food, cupcake, vegan

anawesomeshot, theperfectphotographer, flash, damniwishidtakenthat, spiritofphotography

nikon, green, light, photoshop, apple, d70

white, yellow, abstract, lines, bus, graphic

sky, geotagged, reflection, cielo, bilbao, reflejo

Huiskes et. al.

Results

- Logistic regression on top-level representation.
- Multimodal Inputs

Mean Average Precision

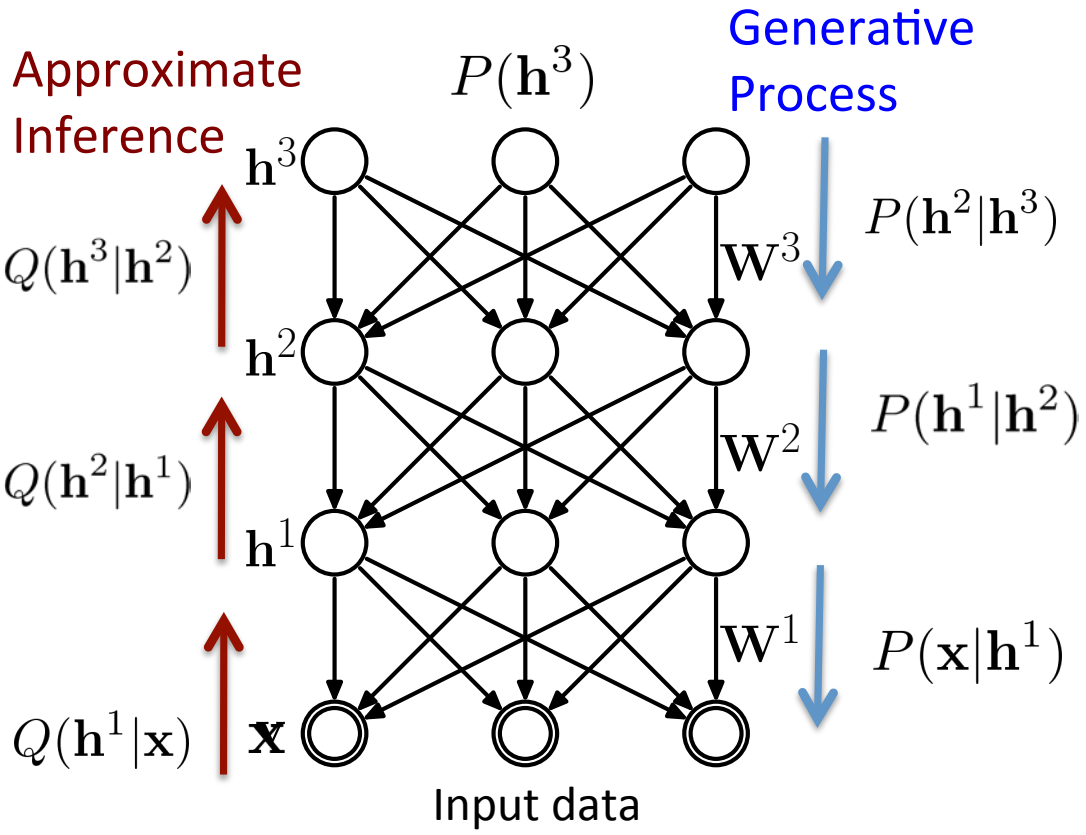
Learning Algorithm	MAP	Precision@50
Random	0.124	0.124
LDA [Huiskes et. al.]	0.492	0.754
SVM [Huiskes et. al.]	0.475	0.758
DBM-Labelled	0.526	0.791
Deep Belief Net	0.638	0.867
Autoencoder	0.638	0.875
DBM	0.641	0.873

Labeled 25K examples

+ 1 Million unlabelled

Helmholtz Machines

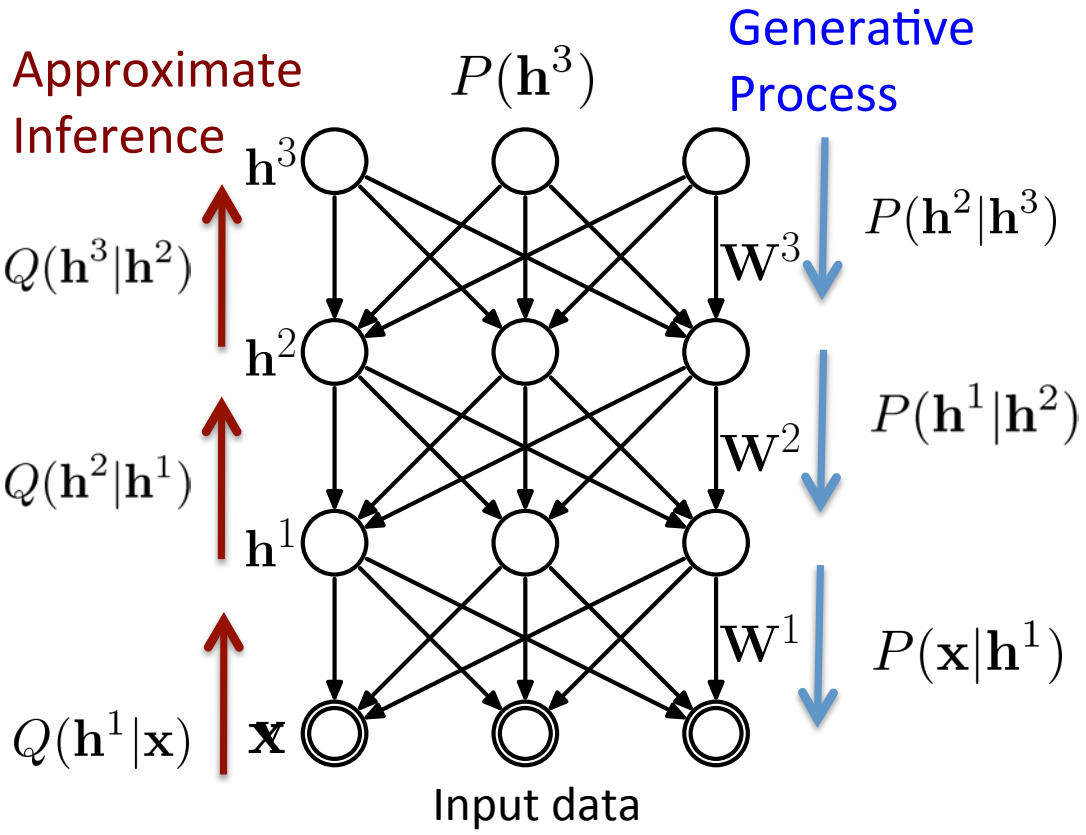
- Hinton, G. E., Dayan, P., Frey, B. J. and Neal, R., Science 1995



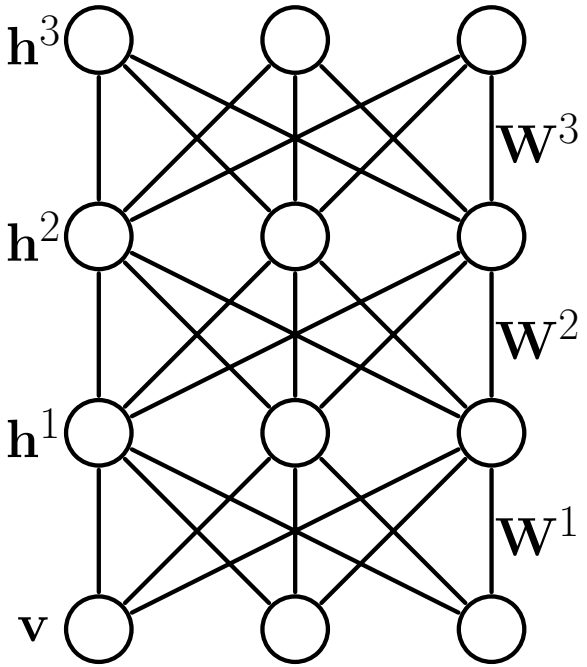
- Kingma & Welling, 2014
- Rezende, Mohamed, Daan, 2014
- Mnih & Gregor, 2014
- Bornschein & Bengio, 2015
- Tang & Salakhutdinov, 2013

Helmholtz Machines vs. DBMs

Helmholtz Machine



Deep Boltzmann Machine

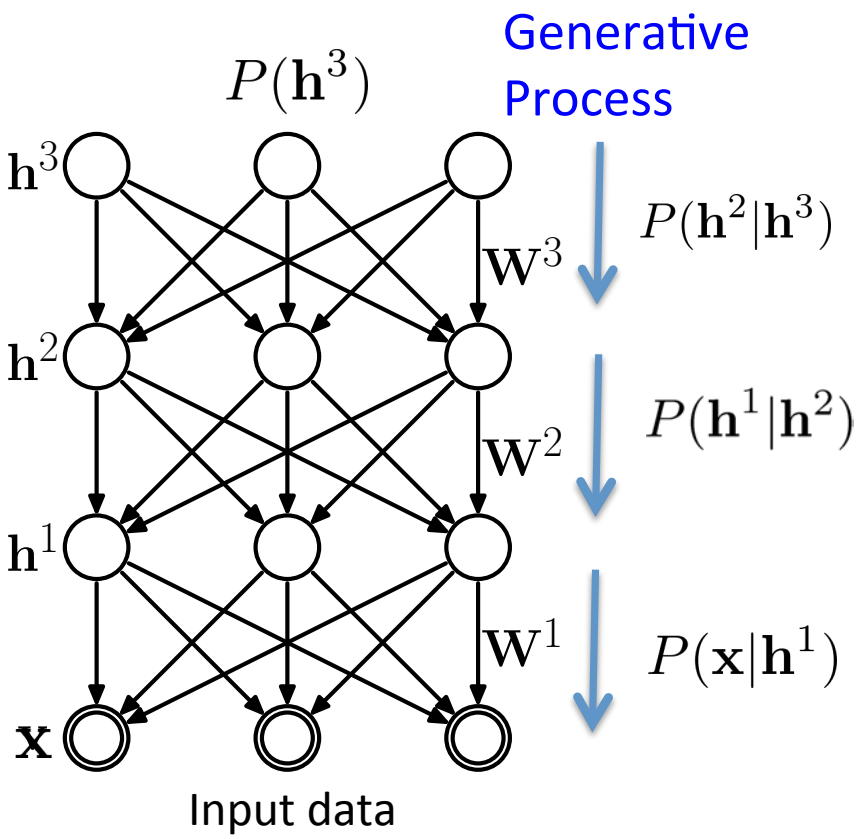


Variational Autoencoders (VAEs)

• The VAE defines a generative process in terms of ancestral sampling through a cascade of hidden stochastic layers:

$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{\mathbf{h}^1,\ldots,\mathbf{h}^L} p(\mathbf{h}^L|\boldsymbol{\theta})p(\mathbf{h}^{L-1}|\mathbf{h}^L,\boldsymbol{\theta})\cdots p(\mathbf{x}|\mathbf{h}^1,\boldsymbol{\theta})$$

Each term may denote a complicated nonlinear relationship



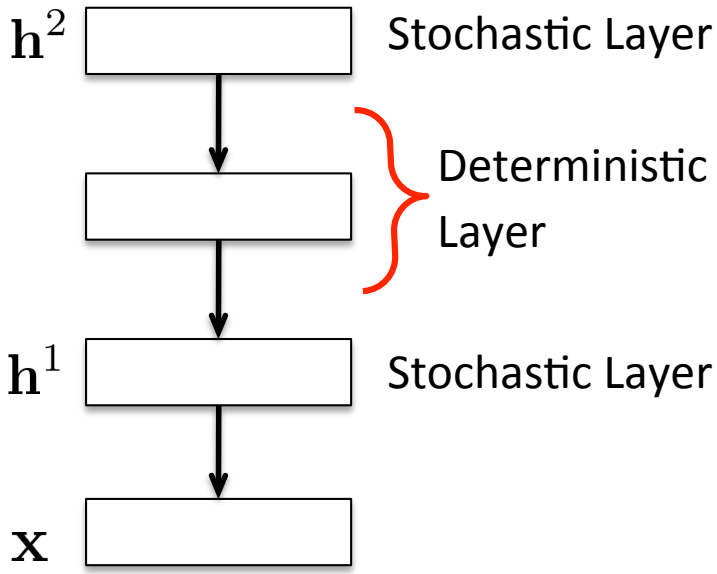
- $\boldsymbol{\theta}$ denotes parameters of VAE.
- L is the number of **stochastic** layers.
- Sampling and probability evaluation is tractable for each $p(\mathbf{h}^\ell|\mathbf{h}^{\ell+1})$.

VAE: Example

• The VAE defines a generative process in terms of ancestral sampling through a cascade of hidden stochastic layers:

$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{\mathbf{h}^1,\mathbf{h}^2} p(\mathbf{h}^2|\boldsymbol{\theta})p(\mathbf{h}^1|\mathbf{h}^2,\boldsymbol{\theta})p(\mathbf{x}|\mathbf{h}^1,\boldsymbol{\theta})$$

This term denotes a one-layer neural net.



- $\boldsymbol{\theta}$ denotes parameters of VAE.
- L is the number of **stochastic** layers.
- Sampling and probability evaluation is tractable for each $p(\mathbf{h}^\ell|\mathbf{h}^{\ell+1})$.

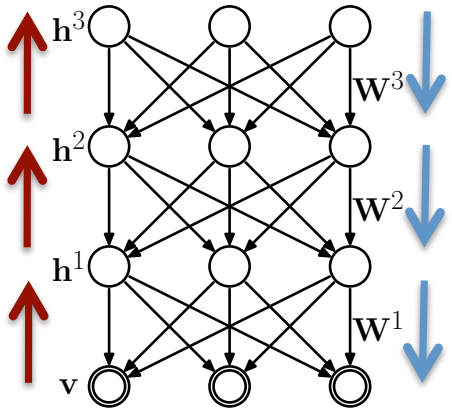
Variational Bound

- The VAE is trained to maximize the variational lower bound:

$$\log p(\mathbf{x}) = \log \mathbb{E}_{q(\mathbf{h}|\mathbf{x})} \left[\frac{p(\mathbf{x}, \mathbf{h})}{q(\mathbf{h}|\mathbf{x})} \right] \geq \mathbb{E}_{q(\mathbf{h}|\mathbf{x})} \left[\log \frac{p(\mathbf{x}, \mathbf{h})}{q(\mathbf{h}|\mathbf{x})} \right] = \mathcal{L}(\mathbf{x})$$

$$\mathcal{L}(\mathbf{x}) = \log p(\mathbf{x}) - \mathrm{D}_{\mathrm{KL}} \left(q(\mathbf{h}|\mathbf{x}) || p(\mathbf{h}|\mathbf{x}) \right)$$

- Trading off the data log-likelihood and the KL divergence from the true posterior.



Input data

- Hard to optimize the variational bound with respect to the recognition network (high-variance).
- Key idea of Kingma and Welling is to use reparameterization trick.

Reparameterization Trick

- Assume that the recognition distribution is Gaussian:

$$q(\mathbf{h}^{\ell}|\mathbf{h}^{\ell-1},\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}(\mathbf{h}^{\ell-1},\boldsymbol{\theta}),\boldsymbol{\Sigma}(\mathbf{h}^{\ell-1},\boldsymbol{\theta}))$$

with mean and covariance computed from the state of the hidden units at the previous layer.

- Alternatively, we can express this in term of auxiliary variable:

$$\boldsymbol{\epsilon}^{\ell} \sim \mathcal{N}(\mathbf{0},\boldsymbol{I})$$

$$\mathbf{h}^{\ell}\left(\boldsymbol{\epsilon}^{\ell},\mathbf{h}^{\ell-1},\boldsymbol{\theta}\right) = \boldsymbol{\Sigma}(\mathbf{h}^{\ell-1},\boldsymbol{\theta})^{1/2}\boldsymbol{\epsilon}^{\ell} + \boldsymbol{\mu}(\mathbf{h}^{\ell-1},\boldsymbol{\theta})$$

Reparameterization Trick

- Assume that the recognition distribution is Gaussian:

$$q(\mathbf{h}^\ell|\mathbf{h}^{\ell-1},\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}(\mathbf{h}^{\ell-1},\boldsymbol{\theta}),\boldsymbol{\Sigma}(\mathbf{h}^{\ell-1},\boldsymbol{\theta}))$$

- Or

$$\boldsymbol{\epsilon}^\ell \sim \mathcal{N}(\mathbf{0},\boldsymbol{I})$$

$$\mathbf{h}^\ell\left(\boldsymbol{\epsilon}^\ell,\mathbf{h}^{\ell-1},\boldsymbol{\theta}\right) = \boldsymbol{\Sigma}(\mathbf{h}^{\ell-1},\boldsymbol{\theta})^{1/2}\boldsymbol{\epsilon}^\ell + \boldsymbol{\mu}(\mathbf{h}^{\ell-1},\boldsymbol{\theta})$$

- The recognition distribution $q(\mathbf{h}^\ell|\mathbf{h}^{\ell-1},\boldsymbol{\theta})$ can be expressed in terms of a deterministic mapping:

$$\underbrace{\mathbf{h}\left(\boldsymbol{\epsilon},\mathbf{x},\boldsymbol{\theta}\right)}, \quad \text{with} \quad \boldsymbol{\epsilon} = \underbrace{(\boldsymbol{\epsilon}^1,\ldots,\boldsymbol{\epsilon}^L)}$$

Deterministic Encoder

Distribution of $\boldsymbol{\epsilon}$ does not depend on $\boldsymbol{\theta}$

Computing the Gradients

- The gradient w.r.t the parameters: both recognition and generative:

$$\nabla_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{h} \sim q(\mathbf{h}|\mathbf{x},\boldsymbol{\theta})} \left[\log \frac{p(\mathbf{x}, \mathbf{h}|\boldsymbol{\theta})}{q(\mathbf{h}|\mathbf{x}, \boldsymbol{\theta})} \right]$$

Autoencoder

$$= \nabla_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{\epsilon}^1, \ldots, \boldsymbol{\epsilon}^L \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})} \left[\log \frac{p(\mathbf{x}, \mathbf{h}(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\theta})|\boldsymbol{\theta})}{q(\mathbf{h}(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\theta})|\mathbf{x}, \boldsymbol{\theta})} \right]$$

$$= \mathbb{E}_{\boldsymbol{\epsilon}^1, \ldots, \boldsymbol{\epsilon}^L \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})} \left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\mathbf{x}, \mathbf{h}(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\theta})|\boldsymbol{\theta})}{q(\mathbf{h}(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\theta})|\mathbf{x}, \boldsymbol{\theta})} \right]$$

Gradients can be computed by backprop

The mapping **h** is a deterministic neural net for fixed $\boldsymbol{\epsilon}$.

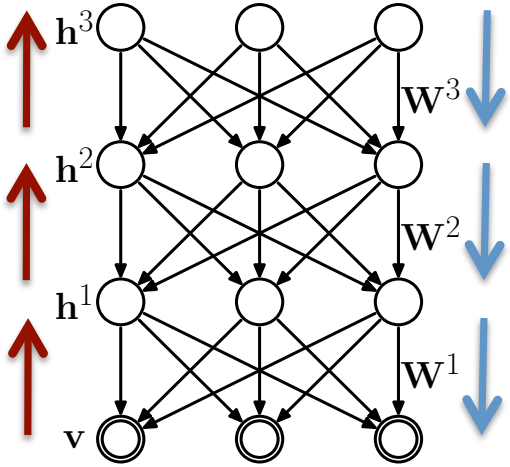
Importance Weighted Autoencoders

- Can improve VAE by using following k-sample importance weighting of the log-likelihood:

$$\mathcal{L}_k(\mathbf{x}) = \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_k \sim q(\mathbf{h}|\mathbf{x})}\left[\log \frac{1}{k}\sum_{i=1}^{k} \frac{p(\mathbf{x},\mathbf{h}_i)}{q(\mathbf{h}_i|\mathbf{x})}\right]$$

$$= \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_k \sim q(\mathbf{h}|\mathbf{x})}\left[\log \frac{1}{k}\sum_{i=1}^{k} w_i\right]$$

unnormalized importance weights

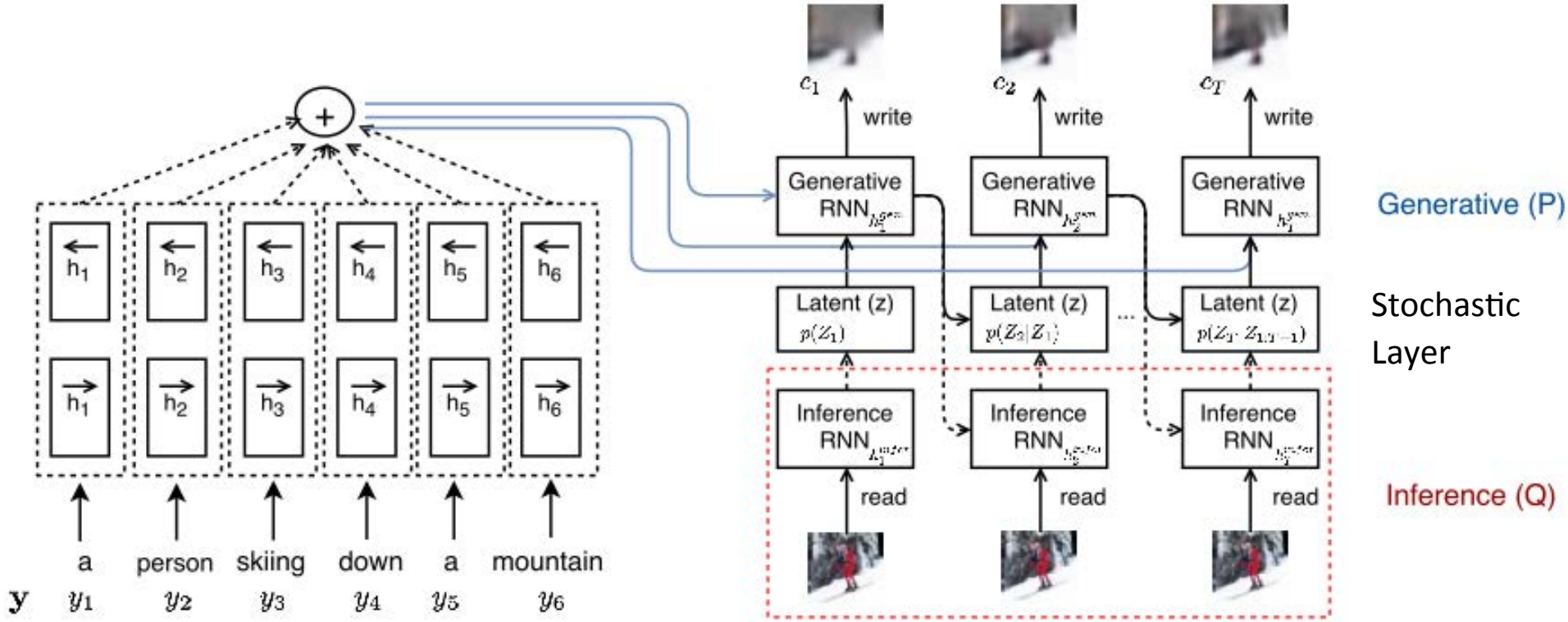


Input data

where $\mathbf{h}_1, \ldots, \mathbf{h}_k$ are sampled from the recognition network.

Burda, Grosse, Salakhutdinov, 2015

Generating Images from Captions



- Generative Model: Stochastic Recurrent Network, chained sequence of Variational Autoencoders, with a single stochastic layer.
- Recognition Model: Deterministic Recurrent Network.

Gregor et. al. 2015

(Mansimov, Parisotto, Ba, Salakhutdinov, 2015)

Motivating Example

- Can we generate images from natural language descriptions?

A **stop sign** is flying in blue skies

A **pale yellow school bus** is flying in blue skies

A **herd of elephants** is flying in blue skies

A **large commercial airplane** is flying in blue skies

(Mansimov, Parisotto, Ba, Salakhutdinov, 2015)

Flipping Colors

A **yellow school bus** parked in the parking lot

A **red school bus** parked in the parking lot

A **green school bus** parked in the parking lot

A **blue school bus** parked in the parking lot

(Mansimov, Parisotto, Ba, Salakhutdinov, 2015)

Novel Scene Compositions

A toilet seat sits open in the bathroom

A toilet seat sits open in the grass field

Ask Google?

(Some) Open Problems

- Reasoning, Attention, and Memory
- Natural Language Understanding
- Deep Reinforcement Learning
- Unsupervised Learning / Transfer Learning / One-Shot Learning

(Some) Open Problems

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Who-Did-What Dataset

- **Document**: "…arrested Illinois governor **Rod Blagojevich** and his chief of staff John Harris on corruption charges … included **Blogojevich** allegedly conspiring to sell or trade the senate seat left vacant by President-elect Barack Obama…"

- **Query**: President-elect Barack Obama said Tuesday he was not aware of alleged corruption by **X** who was arrested on charges of trying to sell Obama's senate seat.

- **Answer**: Rod Blagojevich

Onishi, Wang, Bansal, Gimpel, McAllester, EMNLP, 2016

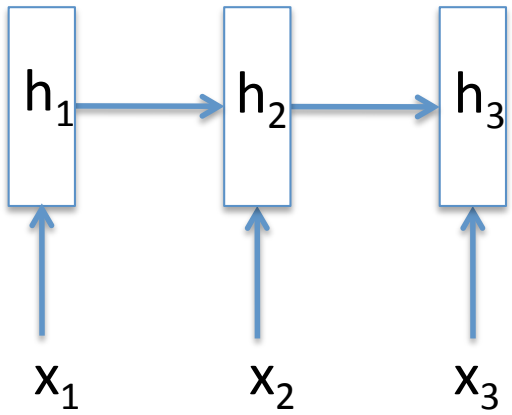
Recurrent Neural Network

$$\mathbf{h_t} = \phi\left(\mathbf{U}\mathbf{h_{t-1}} + \mathbf{W}\mathbf{x_t} + \mathbf{b}\right)$$

Nonlinearity

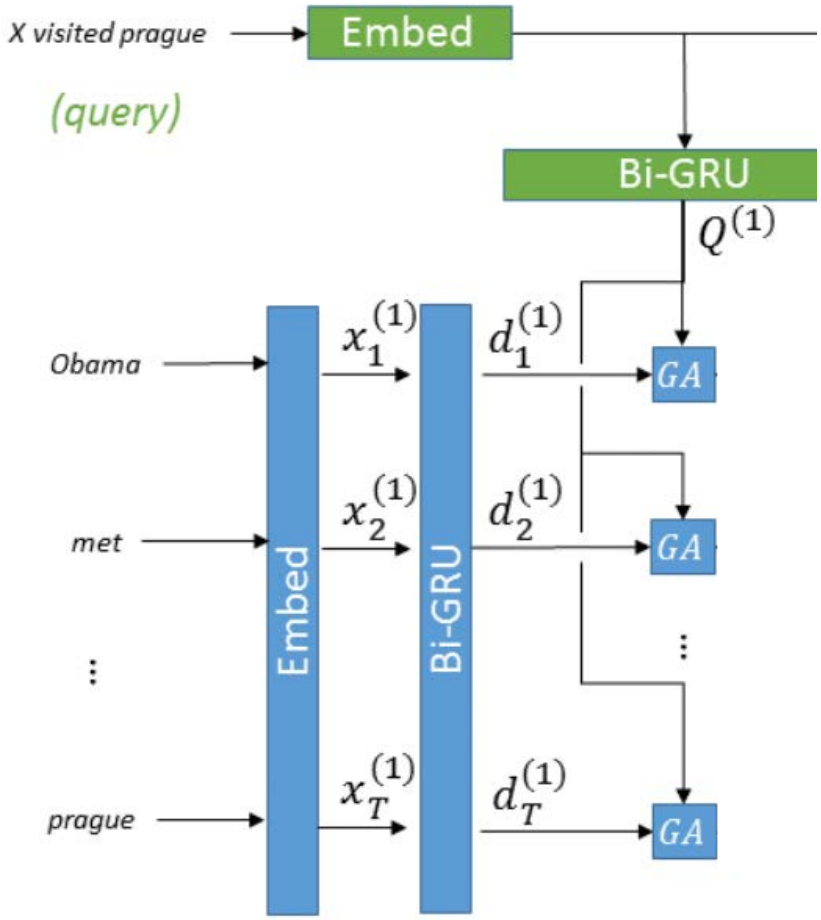
Hidden State at previous time step

Input at time step t



Gated Attention Mechanism

• Use Recurrent Neural Networks (RNNs) to encode a document and a query:



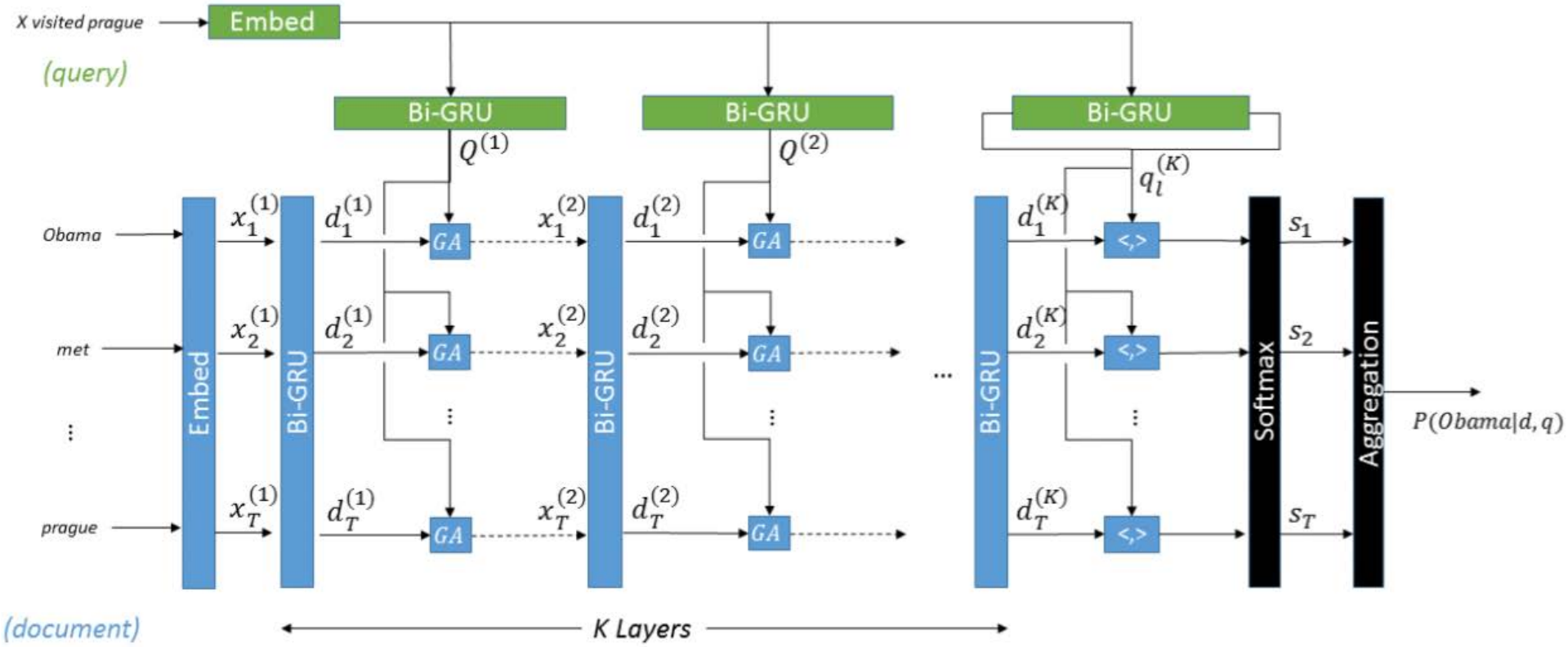
- Use element-wise multiplication to model the interactions between document and query:

$$x_i = d_i \odot q_i$$

(Dhingra, Liu, Yang, Cohen, Salakhutdinov, ACL 2017)

Multi-hop Architecture

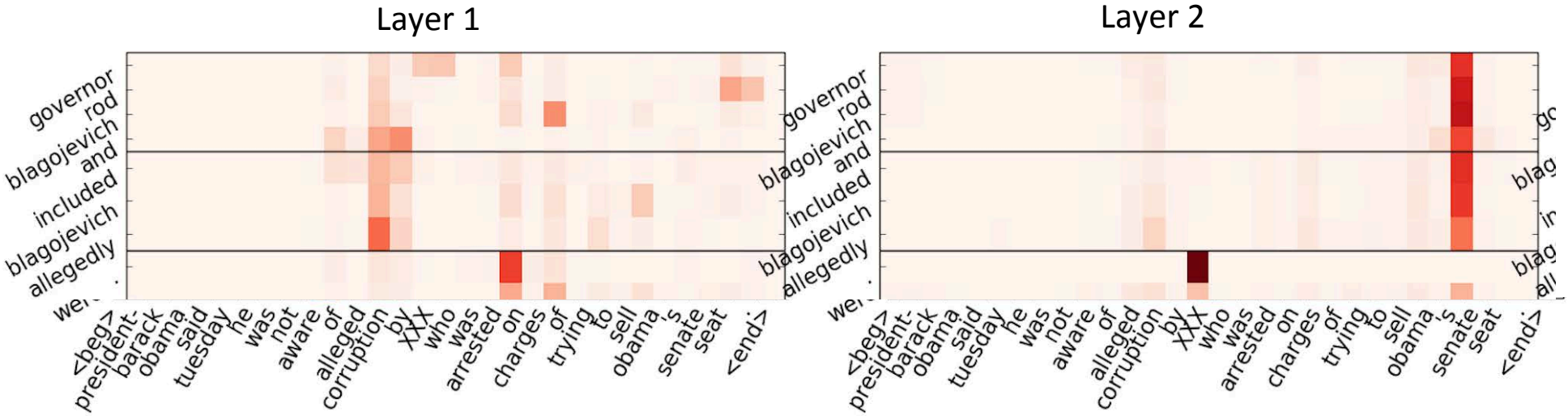
- Reasoning requires several passes over the context



(Dhingra, Liu, Yang, Cohen, Salakhutdinov, ACL 2017)

Analysis of Attention

- **Context**: "…arrested Illinois governor **Rod Blagojevich** and his chief of staff John Harris on corruption charges … included **Blogojevich** allegedly conspiring to sell or trade the senate seat left vacant by President-elect Barack Obama…"
- **Query**: "President-elect Barack Obama said Tuesday he was not aware of alleged corruption by **X** who was arrested on charges of trying to sell Obama's senate seat."
- **Answer**: **Rod Blagojevich**



Analysis of Attention

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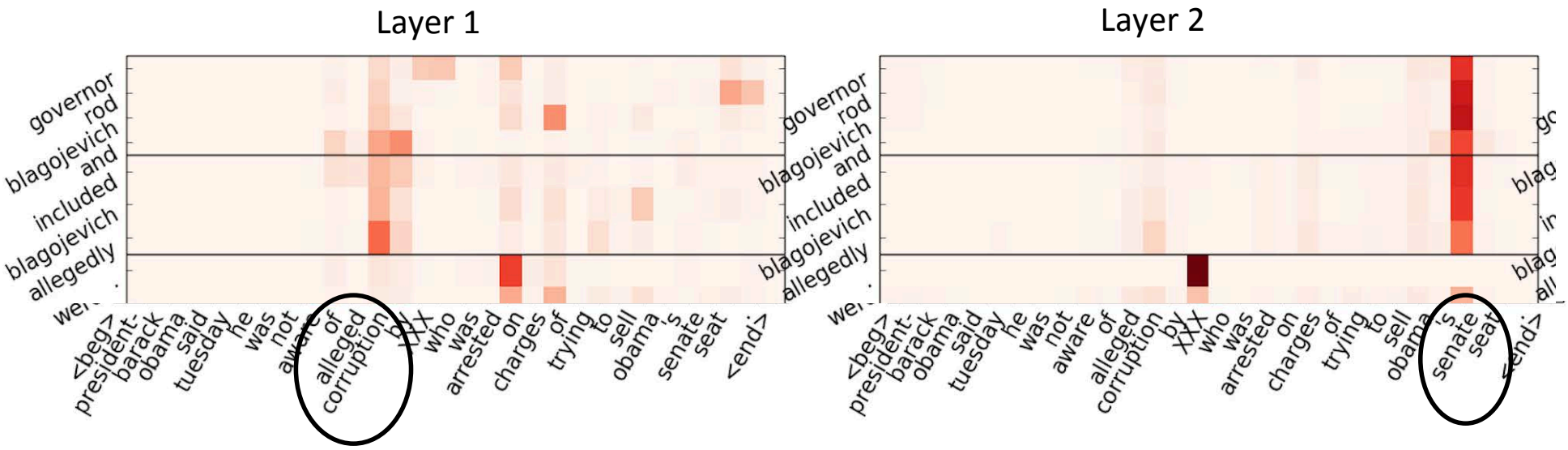
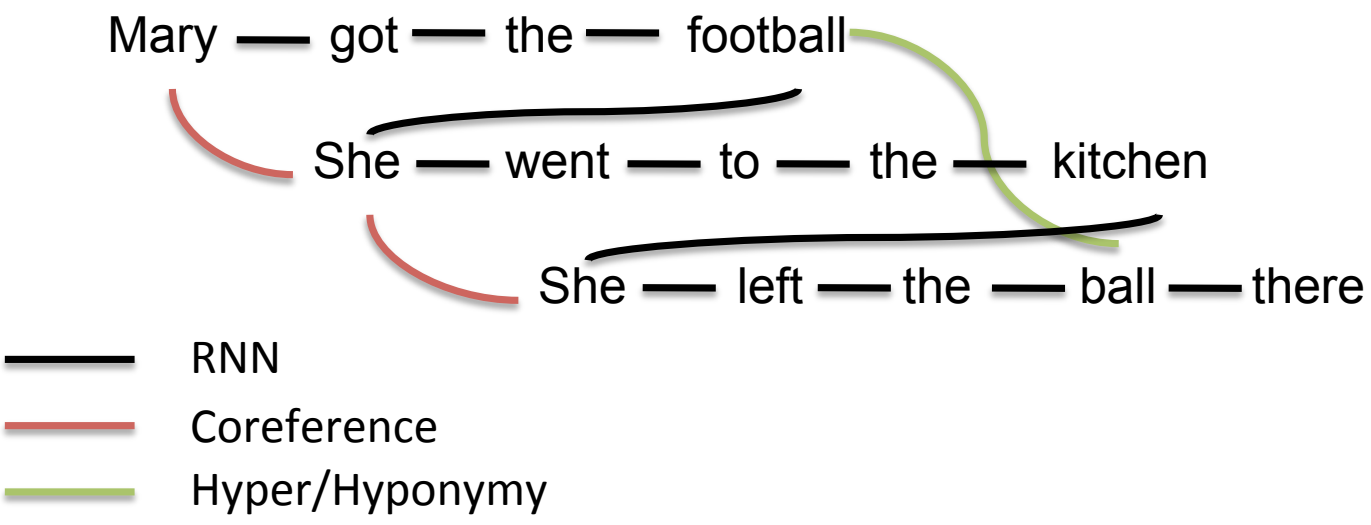


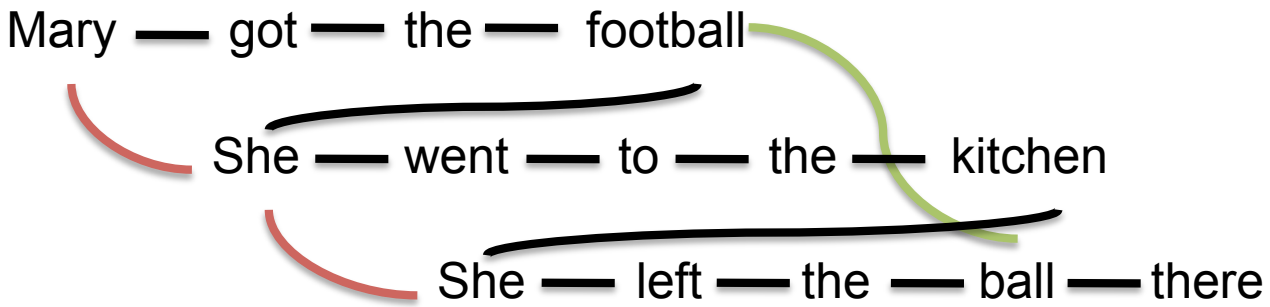
Code + Data: https://github.com/bdhingra/ga-reader

Incorporating Prior Knowledge



Dhingra, Yang, Cohen, Salakhutdinov 2017

Incorporating Prior Knowledge

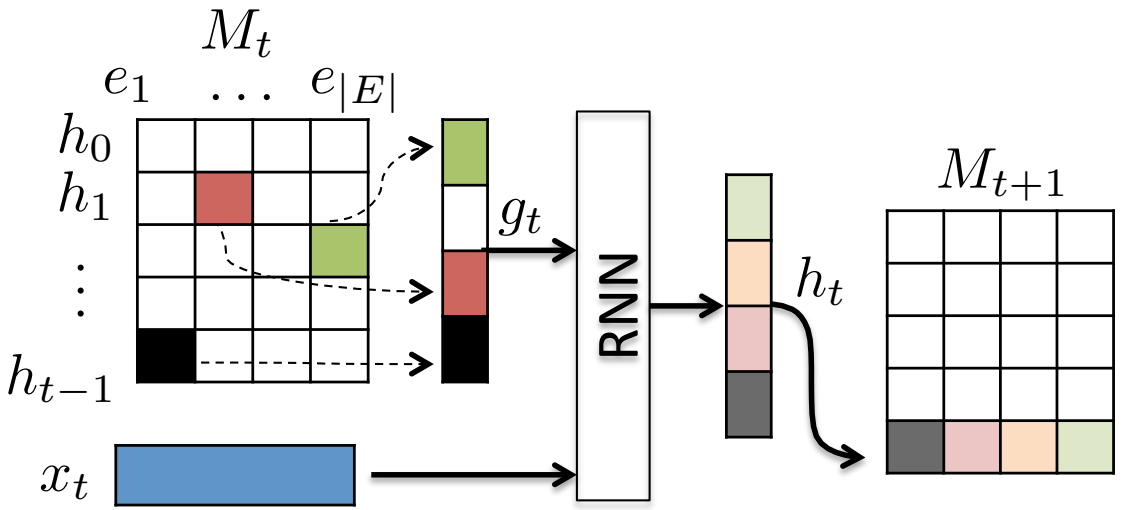


RNN

Coreference

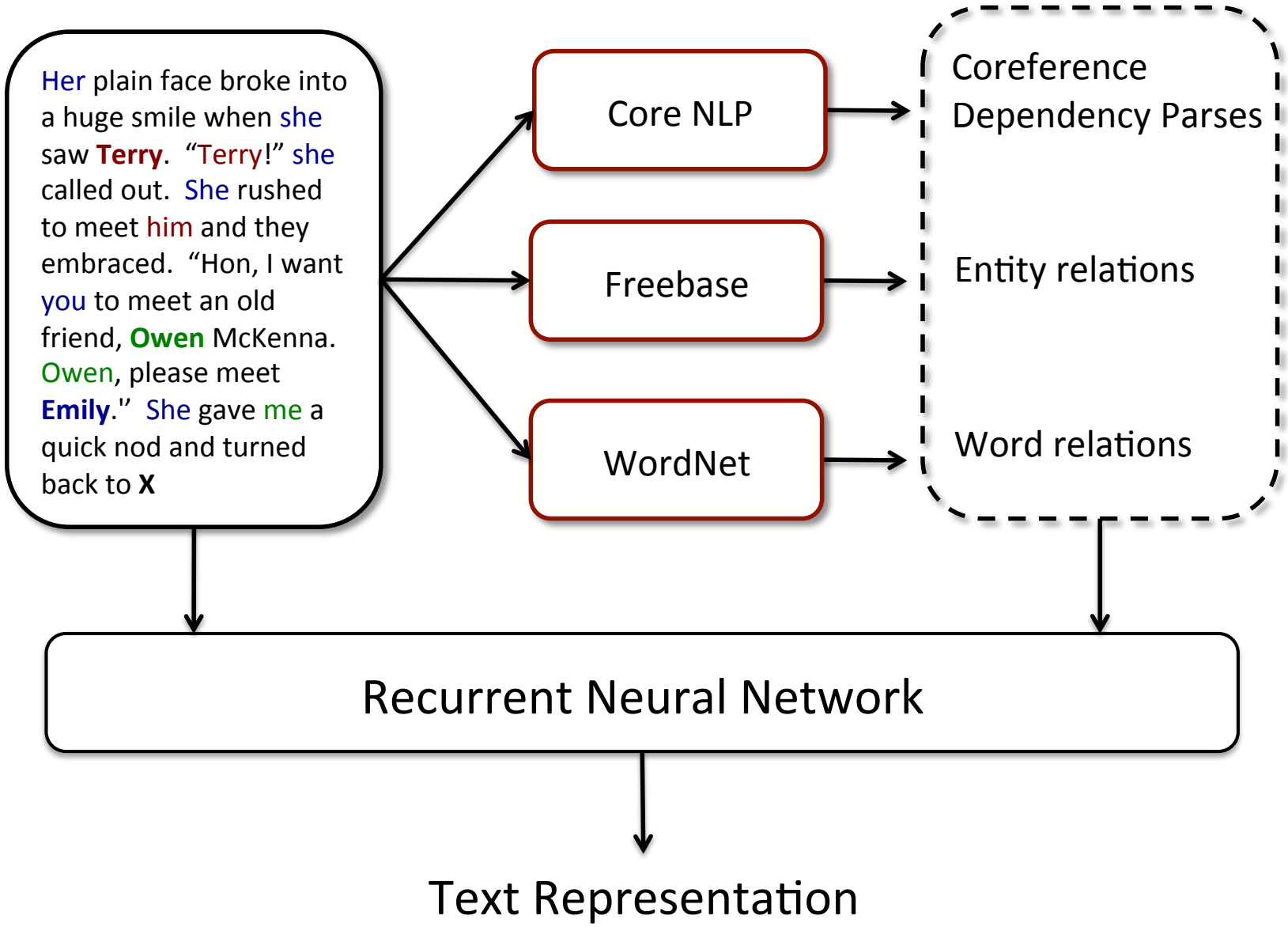
Hyper/Hyponymy

Memory as **A**cyclic **G**raph **E**ncoding (MAGE) - RNN



Dhingra, Yang, Cohen, Salakhutdinov 2017

Incorporating Prior Knowledge



Neural Story Telling

Sample from the Generative Model (recurrent neural network):

She was in love with him for the first time in months, so she had no intention of escaping.

The sun had risen from the ocean, making her feel more alive than normal. She is beautiful, but the truth is that I do not know what to do. The sun was just starting to fade away, leaving people scattered around the Atlantic Ocean.

(Kiros et al., NIPS 2015)

(Some) Open Problems

- Reasoning, Attention, and Memory
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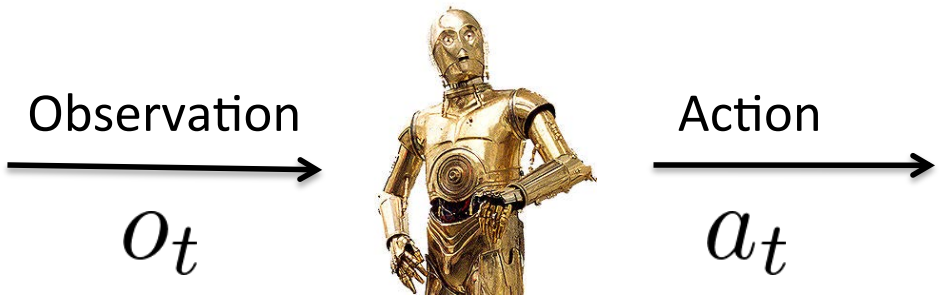
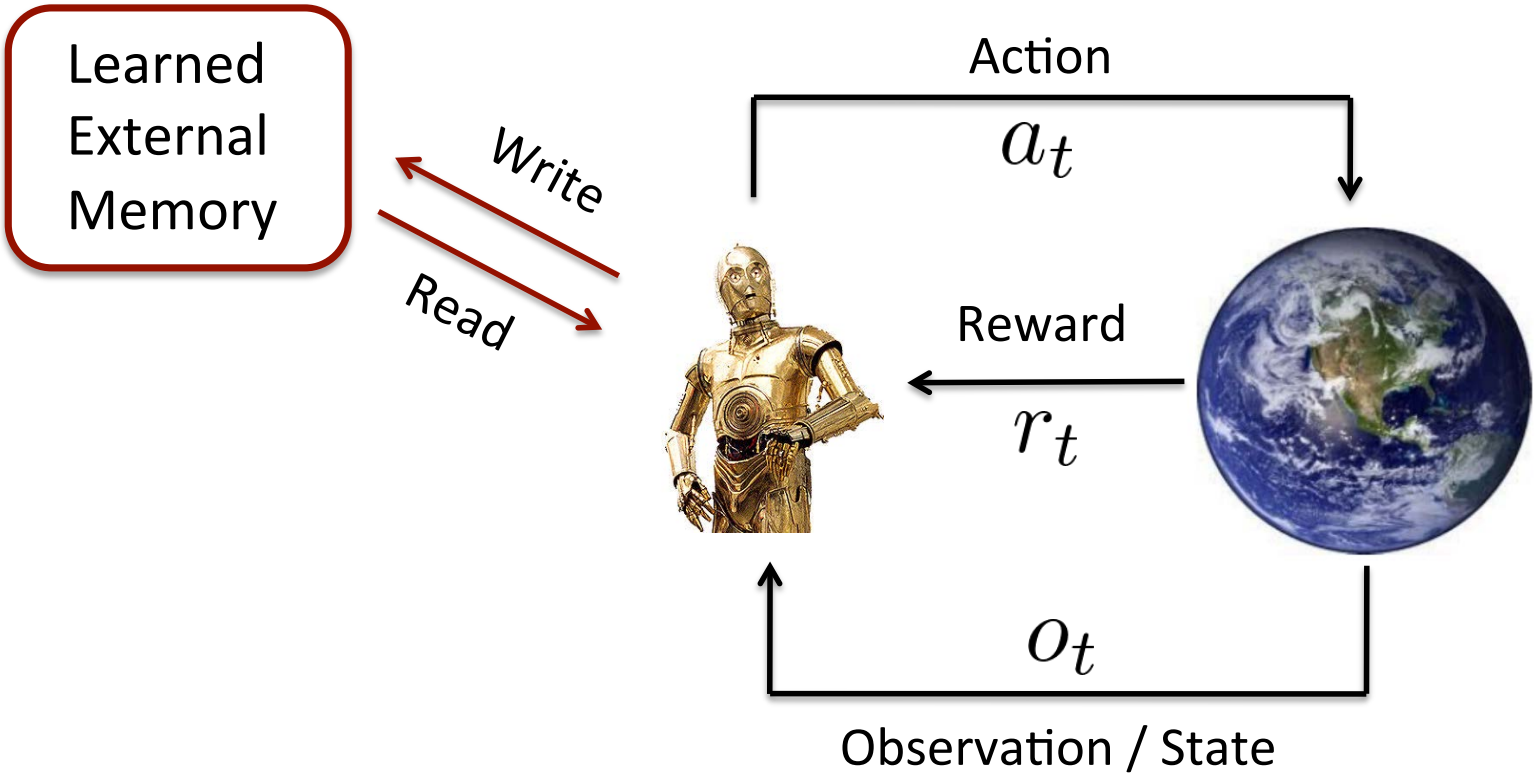
- Unsupervised Learning / Transfer Learning / One-Shot Learning

Learning Behaviors



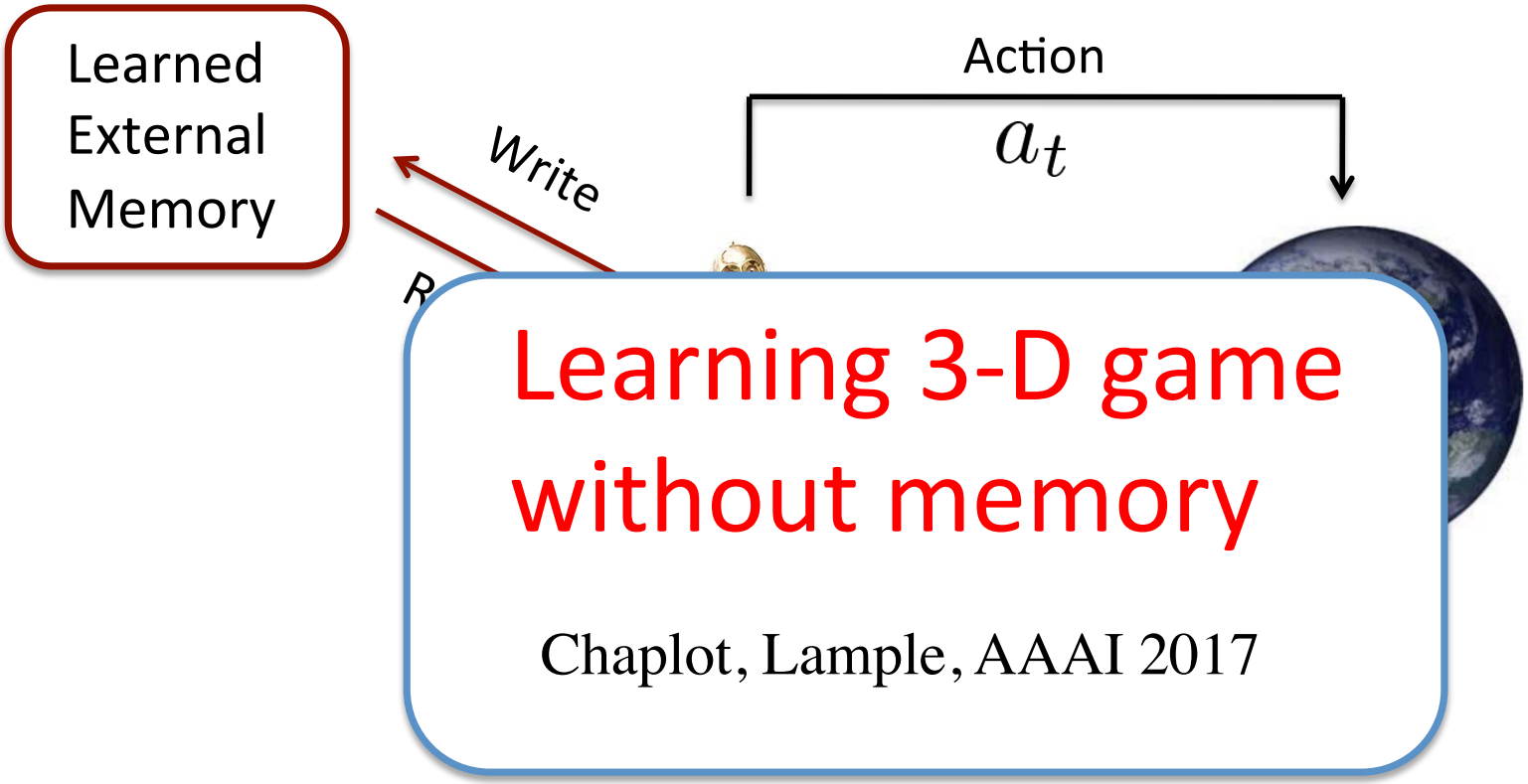
Learning to map sequences of observations to actions, for a particular goal

Reinforcement Learning with Memory



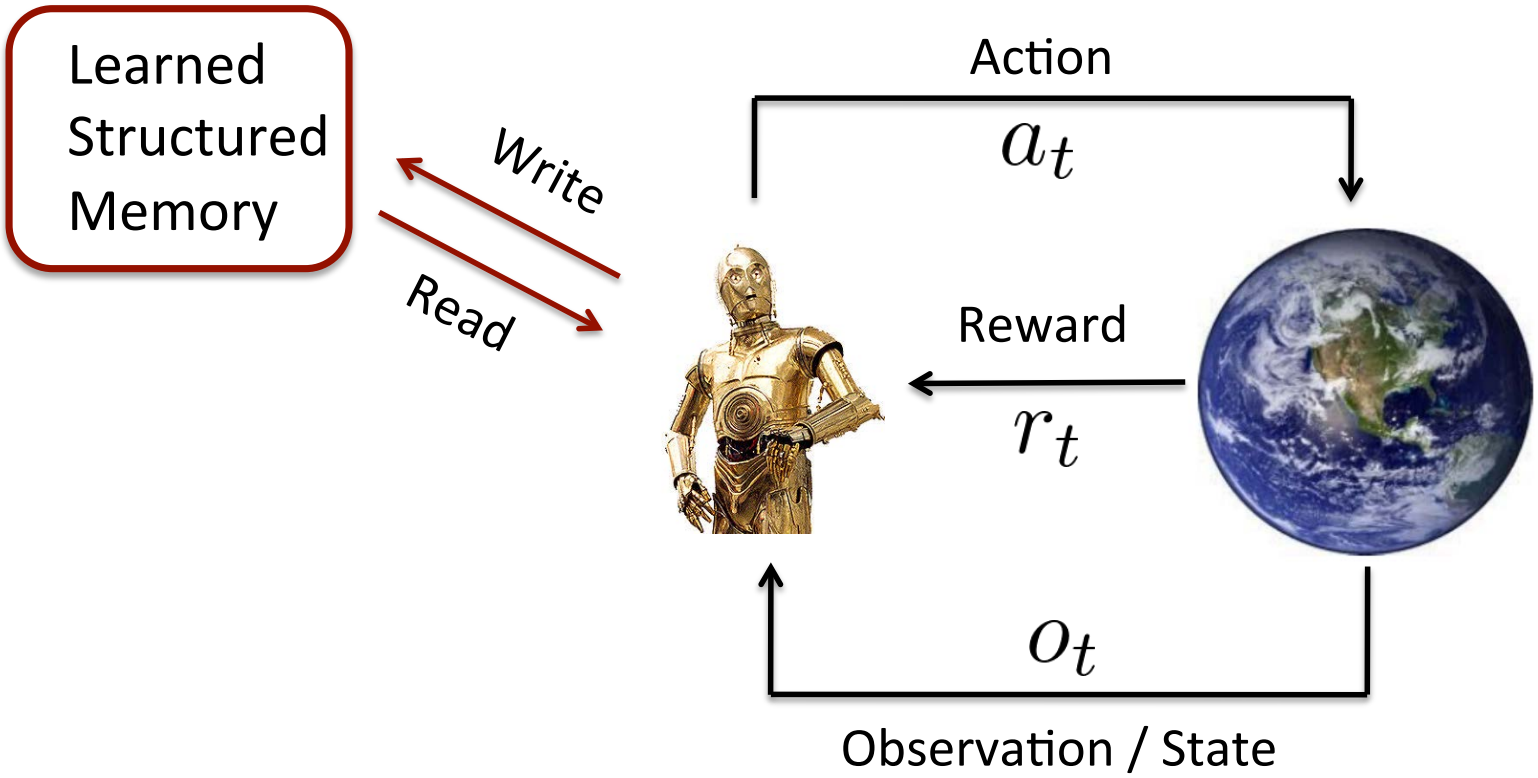
Differentiable Neural Computer, Graves et al., Nature, 2016;
Neural Turing Machine, Graves et al., 2014

Reinforcement Learning with Memory



Differentiable Neural Computer, Graves et al., Nature, 2016;
Neural Turing Machine, Graves et al., 2014

Deep RL with Memory

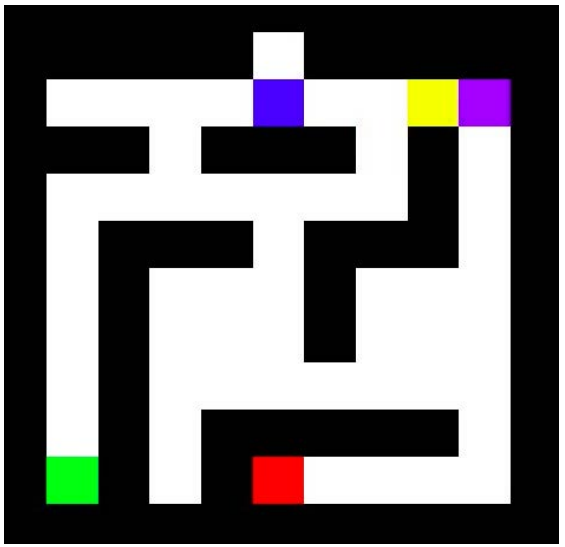


Parisotto, Salakhutdinov, 2017

Random Maze with Indicator

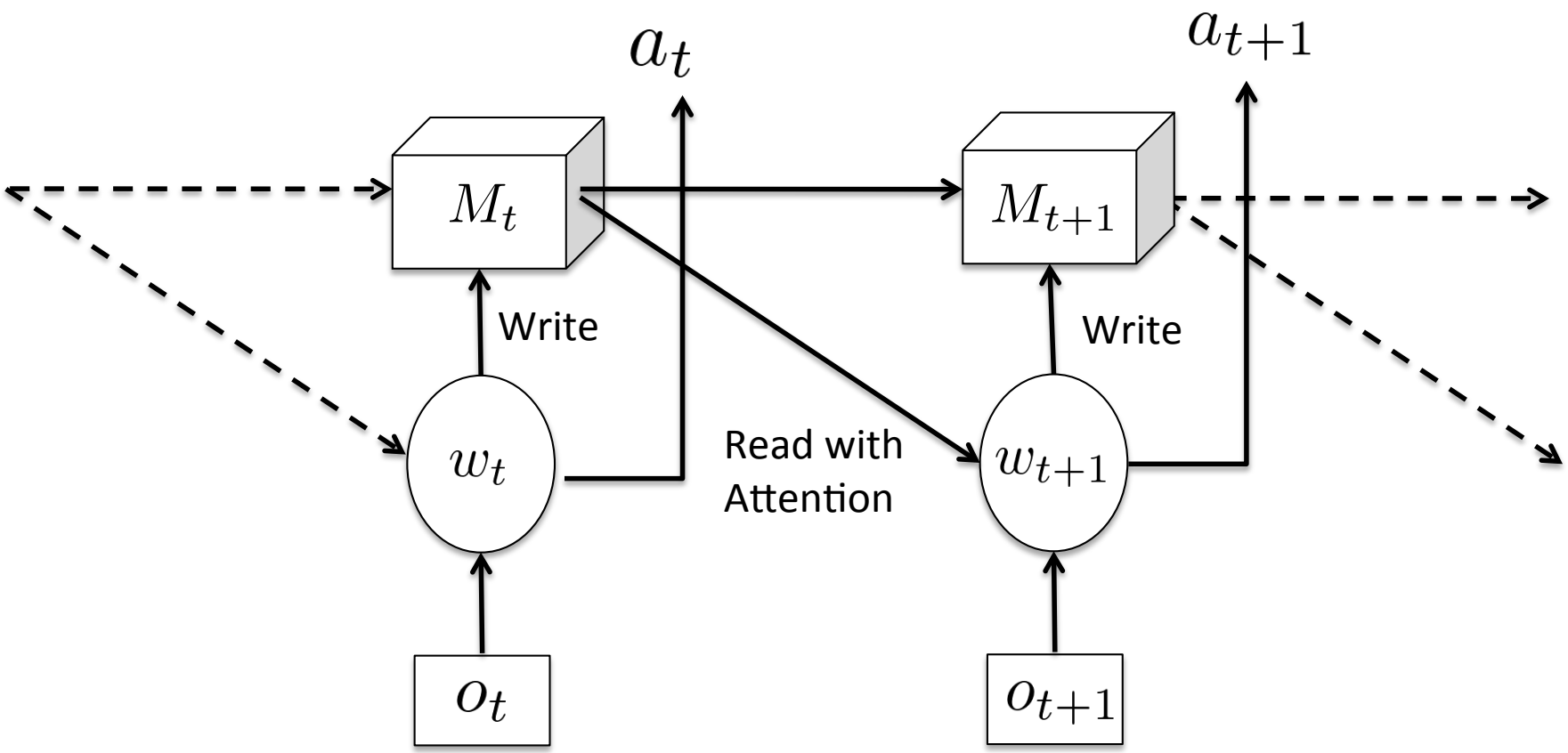
- Indicator: Either blue or pink
  - If blue, find the green block
  - If pink, find the red block

- Negative reward if agent does not find correct block in N steps or goes to wrong block.



Parisotto, Salakhutdinov, 2017

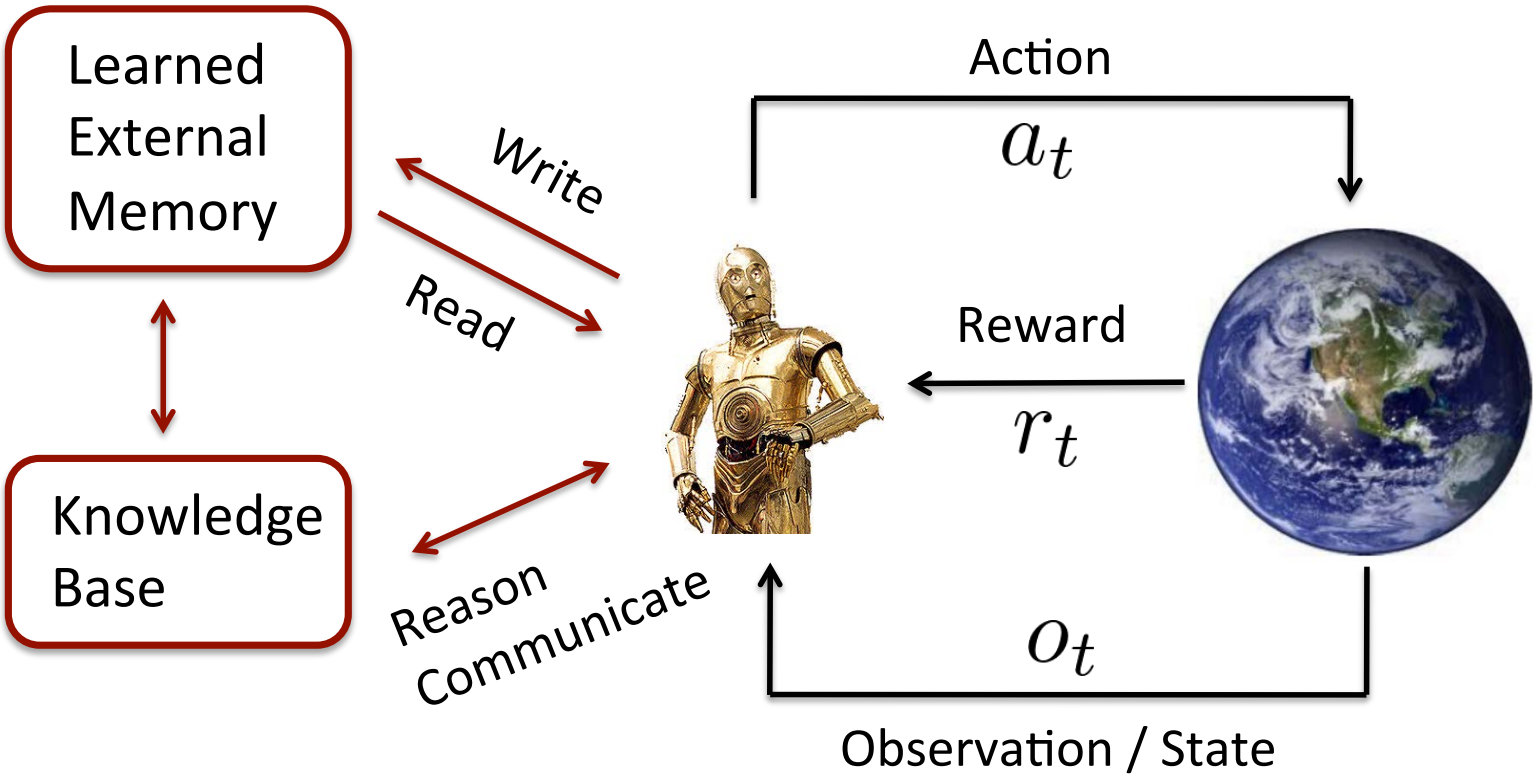
Random Maze with Indicator



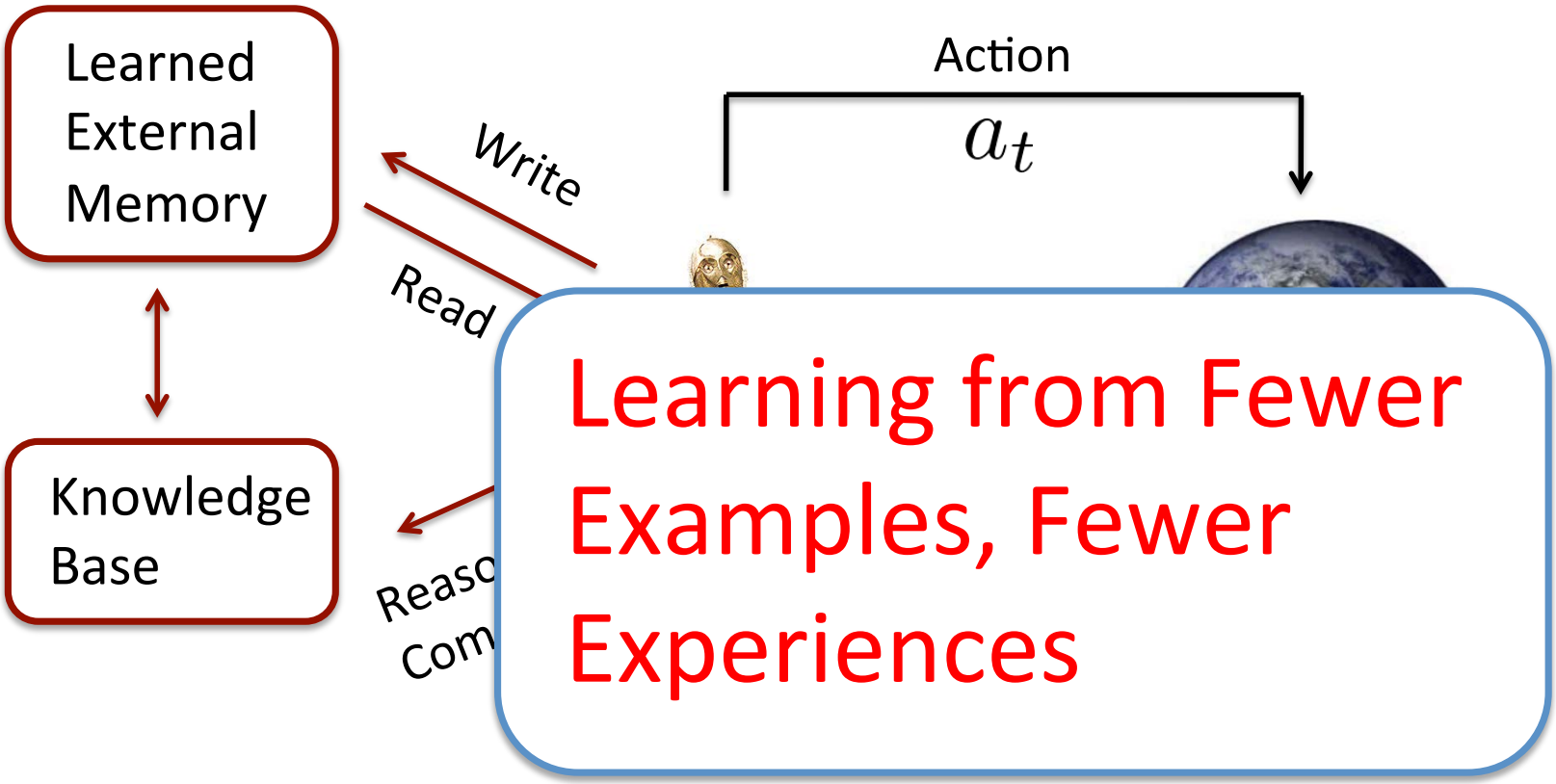
Parisotto, Salakhutdinov, 2017

Random Maze with Indicator

Building Intelligent Agents



Building Intelligent Agents



Summary

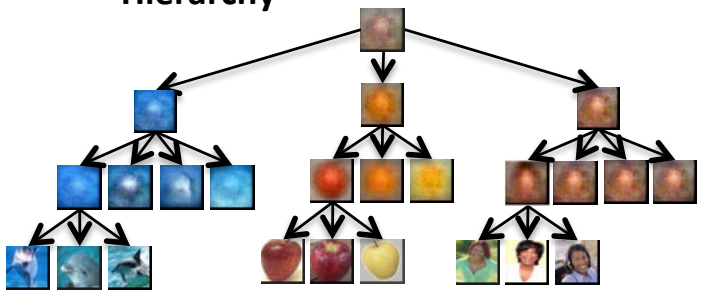
- Efficient learning algorithms for Deep Unsupervised Models

Text & image retrieval / Object recognition

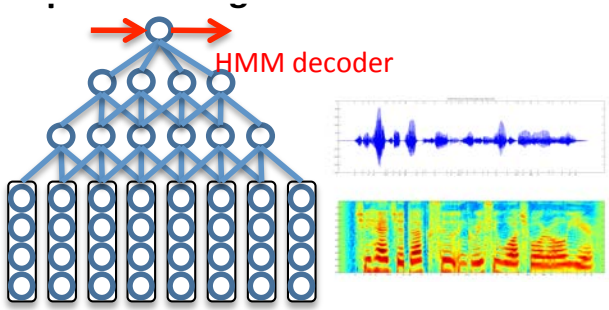
Image Tagging

mosque, tower, building, cathedral, dome, castle

Learning a Category Hierarchy



Object Detection



Multimodal Data

sunset, pacific ocean, beach, seashore

- Deep models improve the current state-of-the art in many application domains:
  - Object recognition and detection, text and image retrieval, handwritten character and speech recognition, and others.

Thank you