智能感知与计算研究中心
Center for Research on Intelligent Perception and Computing

中国科学院自动化研究所
Institute of Automation
Chinese Academy of Sciences

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"Deep Learning Lecture"

Lecture 7: Generative Model (1)

Yan Huang

Center for Research on Intelligent Perception and Computing (CRIPAC)

National Laboratory of Pattern Recognition (NLPR)

Institute of Automation, Chinese Academy of Science (CASIA)

Outline

1. Course Review
2. Linear Factor Model
3. Autoencoder
4. DBN and RBM

Review: Regularization Strategies

- Parameter Norm Penalties
- Dataset Augmentation
- Noise Robustness
- Early Stopping
- Parameter Tying and Parameter Sharing
- Multitask Learning
- Bagging and Other Ensemble Methods
- Dropout
- Adversarial Training

Review: Parameter Norm Penalties

- This approach limits the capacity of the model by adding the penalty Ω (θ) to the objective function resulting in:

$$\tilde{J}(\theta) = J(\theta) + \alpha\Omega(\theta)$$

- $\alpha \in [0,1)$ is a hyper-parameter that weights the relative contribution of the norm penalty to the value of the objective function.
- L2 Norm Parameter Regularization

$$\Omega(\theta) = \frac{1}{2}\|w\|_2^2 = \frac{1}{2}w^T w$$

- L1 Norm Parameter Regularization

$$\Omega(\theta) = ||\mathbf{w}|| = \sum_i |w_i|$$

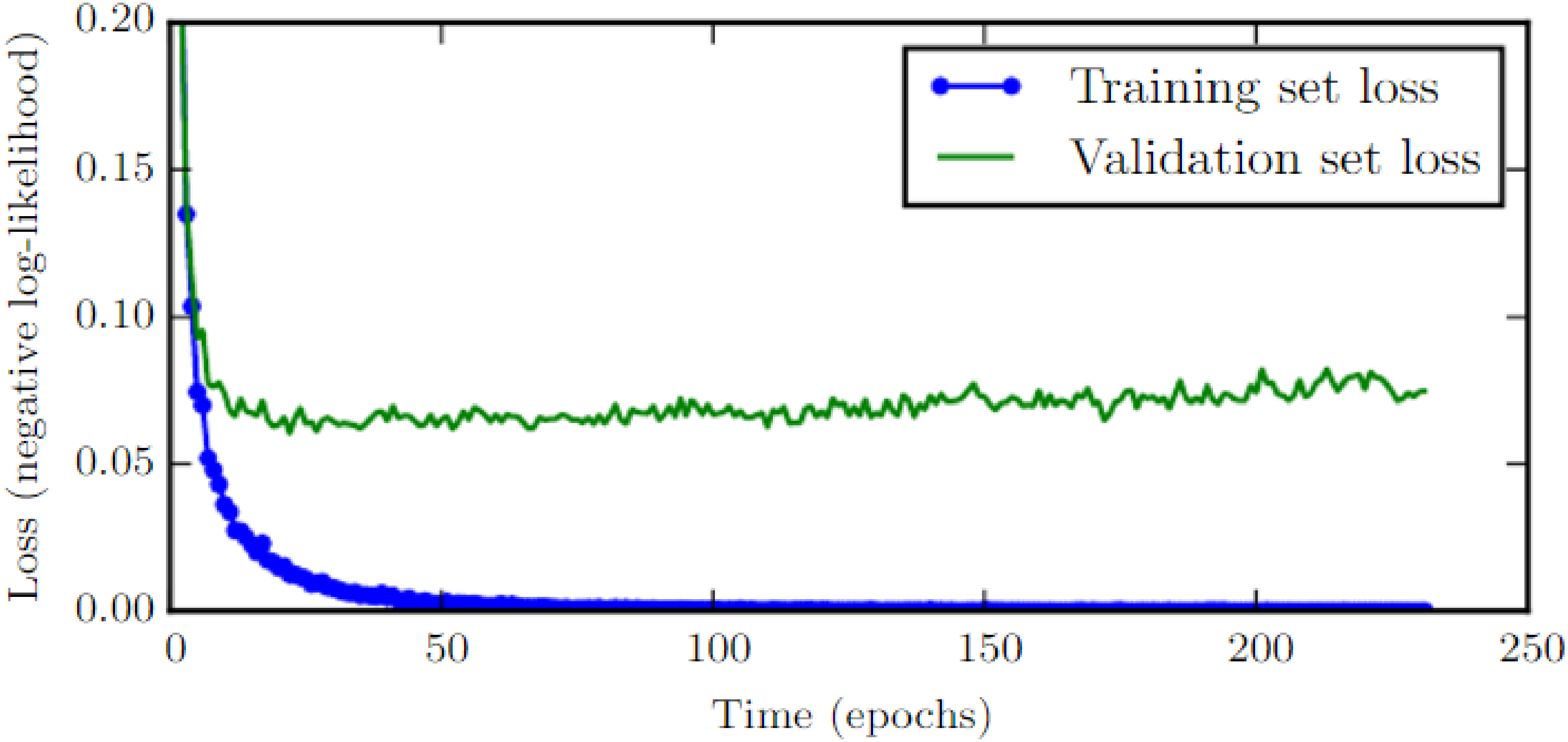
Review: Dataset Augmentation

Color jitter

Horizontal flipping

Relative performance improvement is limited!

Review: Early Stopping



Review: Parameter Sharing and Parameter Tying

- **Parameter Sharing** imposes much stronger assumptions on parameters through forcing the parameter sets to be equal**.**
- Examples would be Siamese networks, convolution operators, and multitask learning.

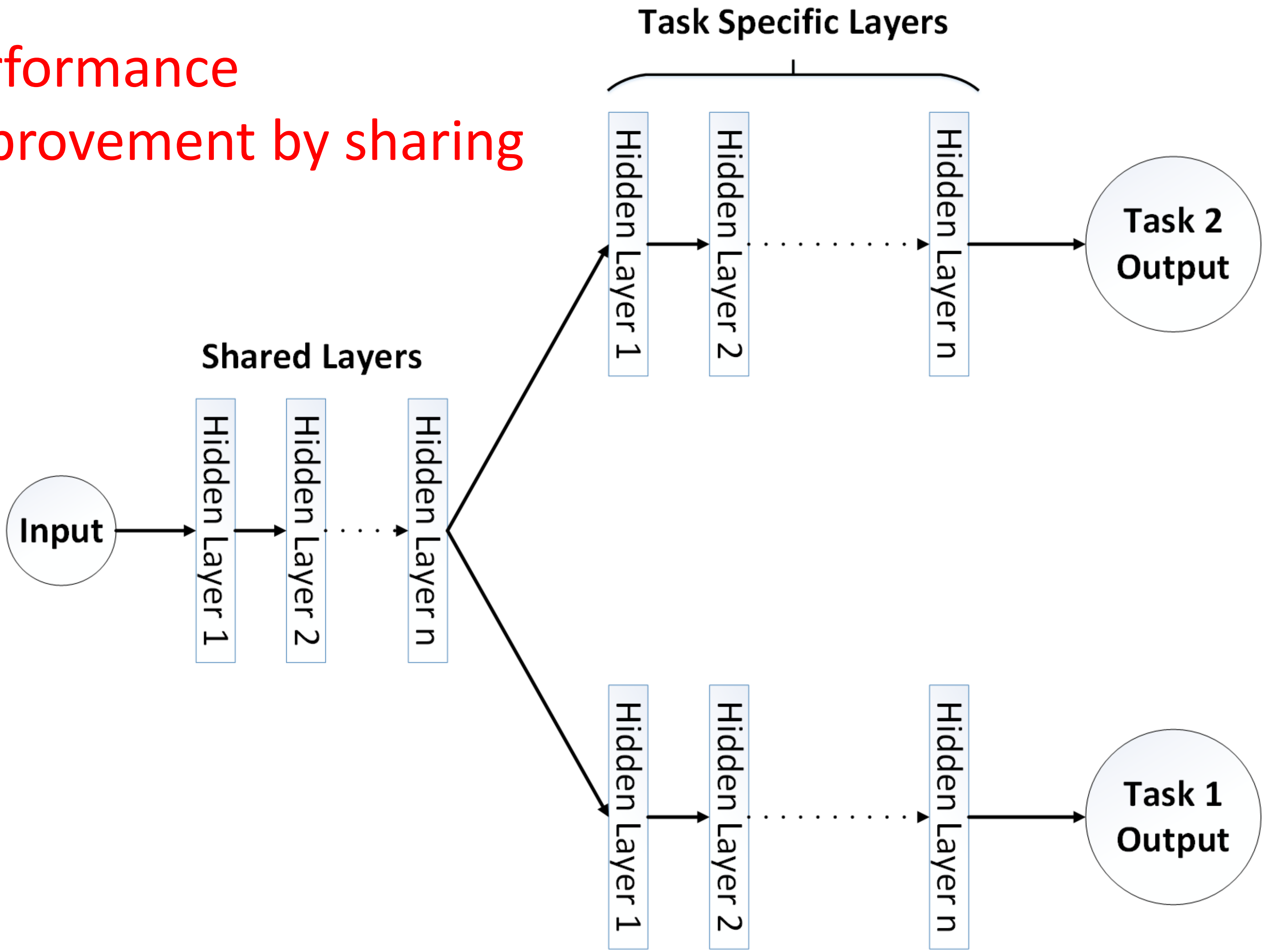
- **Parameter Tying** refers to explicitly forcing the parameters of two models to be close to each other, through the norm penalty:

$$||\mathbf{w}^{(A)} - \mathbf{w}^{(B)}||$$

- Here, $w^{(A)}$ refers to the weights of the first model while $w^{(B)}$ refers to those of the second one.

Review: Multitask Learning

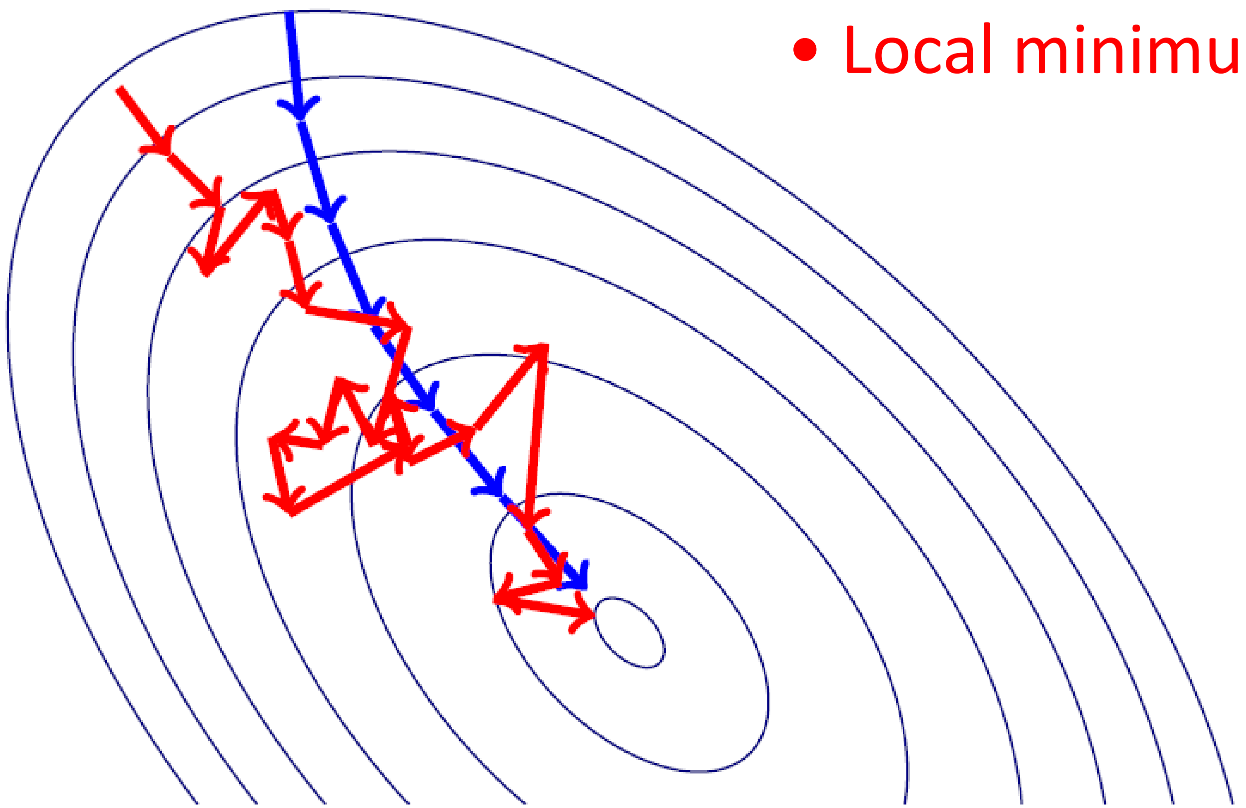
Performance improvement by sharing



Review: Optimization

- Stochastic Gradient Descent
- Momentum Method and the Nesterov Variant
- Adaptive Learning Methods (AdaGrad, RMSProp, Adam)
- Batch Normalization
- Initialization Heuristics

Review: SGD Vs BGD



- Slow convergence
- Local minimum

Review: Comparison

SGD: $\theta \leftarrow \theta - \epsilon\hat{\mathbf{g}}$

Momentum: $\mathbf{v} \leftarrow \alpha\mathbf{v} - \epsilon\hat{\mathbf{g}}$ then $\theta \leftarrow \theta + \mathbf{v}$

Nesterov: $\mathbf{v} \leftarrow \alpha\mathbf{v} - \epsilon\nabla_\theta\left(L(f(\mathbf{x}^{(i)};\theta + \alpha\mathbf{v}), \mathbf{y}^{(i)})\right)$ then $\theta \leftarrow \theta + \mathbf{v}$

AdaGrad: $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$ then $\Delta\theta - \leftarrow \dfrac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$ then $\theta \leftarrow \theta + \Delta\theta$

RMSProp: $\mathbf{r} \leftarrow \rho\mathbf{r} + (1-\rho)\hat{\mathbf{g}} \odot \hat{\mathbf{g}}$ then $\Delta\theta \leftarrow -\dfrac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \hat{\mathbf{g}}$ then $\theta \leftarrow \theta + \Delta\theta$

Adam: $\hat{\mathbf{s}} \leftarrow \dfrac{\mathbf{s}}{1-\rho_1^t}, \hat{\mathbf{r}} \leftarrow \dfrac{\mathbf{r}}{1-\rho_2^t}$ then $\Delta\theta = -\epsilon\dfrac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}}} + \delta}$ then $\theta \leftarrow \theta + \Delta\theta$

Review: Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Why 0-Mean?

"Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift," Ioffe and Szegedy 2015

Outline

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2. Linear Factor Model
3. Autoencoder
4. DBN and RBM

Linear Factor Model

- We want to build a probabilistic model of the input $P(\boldsymbol{x})$
- Like before, we are interested in latent factors **h** that explain **x**
- We then care about the marginal:

$$P(\boldsymbol{x}) = E_{\boldsymbol{h}} P(\boldsymbol{x}|\boldsymbol{h})$$

- The latent factor **h** is an encoding of the data

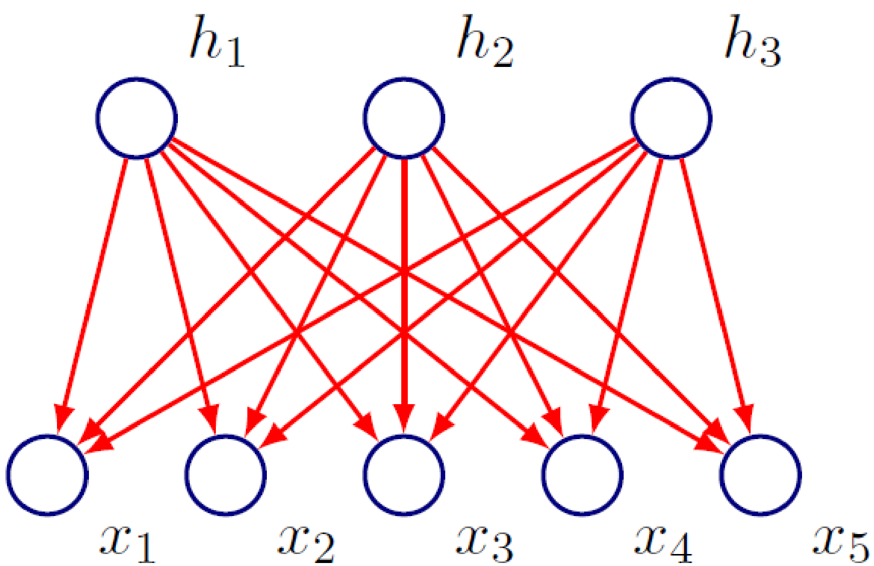
Unsupervised Learning ⇔ Probabilistic Modeling

Linear Factor Model

- Simplest decoding model: Get **x** after a linear transformation of **h** with some noise
- Formally: Suppose we sample the latent factors from a distribution $\mathbf{h} \sim P(\mathbf{h})$
- Then: $\mathbf{x} = W\mathbf{h} + \mathbf{b} + \varepsilon$

Linear Factor Model

- P(**h**) is a factorial distribution



$$\mathbf{x} = W\mathbf{h} + \mathbf{b} + \epsilon$$

- How do learn in such a model?
- Let's look at a simple example

Probabilistic PCA

- Suppose underlying latent factor has a Gaussian distribution

$$\mathbf{h} \sim \mathcal{N}(\mathbf{h}; 0, I)$$

- For the noise model: Assume $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$
- Then:

$$P(\mathbf{x}|\mathbf{h}) = \mathcal{N}(\mathbf{x}|W\mathbf{h} + \mathbf{b}, \sigma^2 I)$$

- We care about the marginal P(x) (predictive distribution):

$$P(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{b}, WW^T + \sigma^2 I)$$

Probabilistic PCA

$$P(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{b}, WW^T + \sigma^2 I)$$

- How do we learn the parameters? (EM, ML Estimation)
- Let's look at the ML Estimation:
  - Let $C = WW^T + \sigma^2 I$
  - We want to maximize $\ell(\theta; X) = \sum_i \log P(\mathbf{x}_i|\theta)$

Probabilistic PCA: ML Estimation

$$\ell(\theta; X) = \sum_i \log P(\mathbf{x}_i|\theta)$$

$$= -\frac{N}{2}\log|C| - \frac{1}{2}\sum_i (\mathbf{x}_i - \mathbf{b})C^{-1}(\mathbf{x}_i - \mathbf{b})^T$$

$$= -\frac{N}{2}\log|C| - \frac{1}{2}Tr[(C^{-1}\sum_i \mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T]$$

$$= \frac{N}{2}\log|C| - \frac{1}{2}Tr[(C^{-1}S]$$

- *S* is the variance matrix: $S = \frac{1}{N}\sum(x_i - b)\,(x_i - b)^T$
- Now fit the parameters θ= W, b, σ to maximize log-likelihood
- Can also use EM

Details can be found in: https://blog.csdn.net/janehong1314/article/details/84918269

Factor Analysis

- Fix the latent factor prior to be the unit Gaussian as before:

$$\mathbf{h} \sim \mathcal{N}(\mathbf{h}; 0, I)$$

- Noise is sampled from a Gaussian with a diagonal covariance:

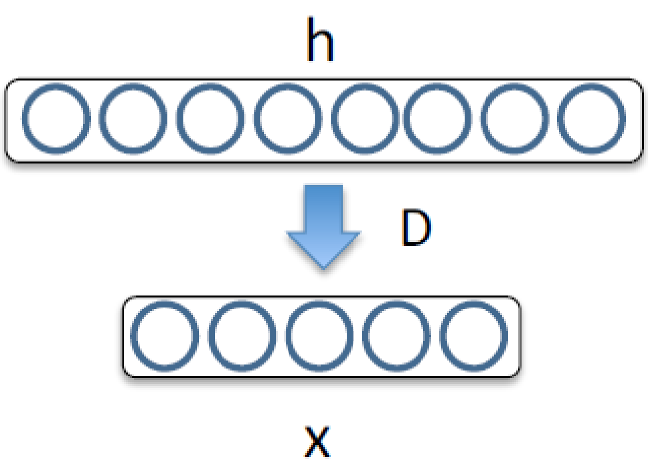
$$\Psi = diag([\sigma_1^2, \sigma_2^2, \ldots, \sigma_d^2])$$

- Still consider linear relationship between inputs and observed variables: Marginal

$$P(\mathbf{x}) \sim \mathcal{N}(\mathbf{x}; b, WW^T + \Psi)$$

Sparse Coding

- Sparse coding (Olshausen & Field, 1996). Originally developed to explain early visual processing in the brain (edge detection).
- For each input $\mathbf{x}^{(t)}$ find a latent representation $\mathbf{h}^{(t)}$ such that:
    - it is sparse: the vector $\mathbf{h}^{(t)}$ has many zeros
    - we can reconstruct the original input $\mathbf{x}^{(t)}$



Sparse Coding

- For each $\mathbf{x}^{(t)}$ find a latent representation $\mathbf{h}^{(t)}$ such that:
  - it is sparse: the vector $\mathbf{h}^{(t)}$ has many zeros
  - we can reconstruct the original input $\mathbf{x}^{(t)}$
- In other words:

Reconstruction: $\widehat{\mathbf{x}}^{(t)}$

Sparsity vs. reconstruction control

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \underbrace{\min_{\mathbf{h}^{(t)}} \frac{1}{2} ||\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}^{(t)}||_2^2}_{\text{Reconstruction error}} + \underbrace{\lambda ||\mathbf{h}^{(t)}||_1}_{\text{Sparsity penalty}}$$

Sparse Coding

- For each $\mathbf{x}^{(t)}$ find a latent representation $\mathbf{h}^{(t)}$ such that:
    - it is sparse: the vector $\mathbf{h}^{(t)}$ has many zeros
    - we can good reconstruct the original input $\mathbf{x}^{(t)}$
- In other words:

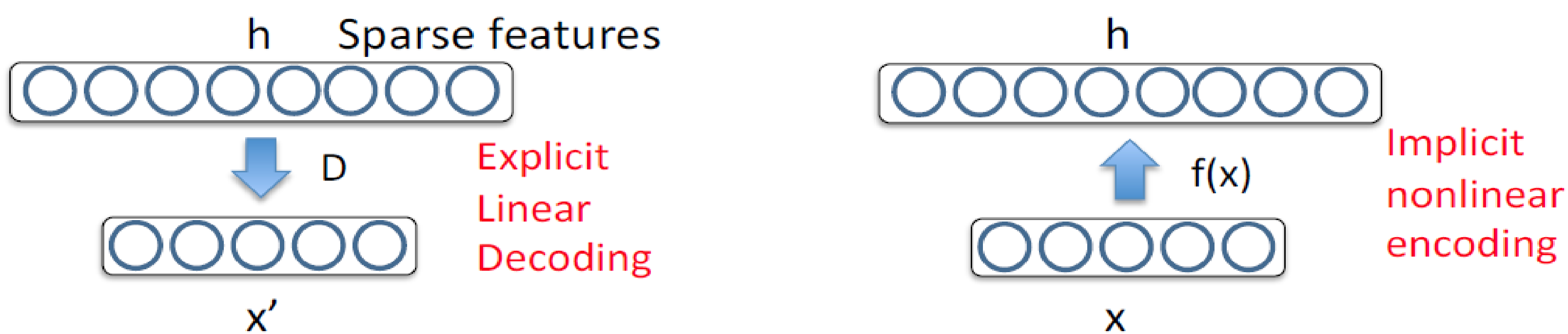
$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} ||\mathbf{x}^{(t)} - \mathbf{D}\, \mathbf{h}^{(t)}||_2^2 + \lambda ||\mathbf{h}^{(t)}||_1$$

    - we also constrain the columns of D to be of norm 1
    - otherwise, D could grow big while h becomes small to satisfy the L1 constraint

Interpreting Sparse Coding

Interpreting Sparse Coding

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} ||\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}^{(t)}||_2^2 + \lambda ||\mathbf{h}^{(t)}||_1$$



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

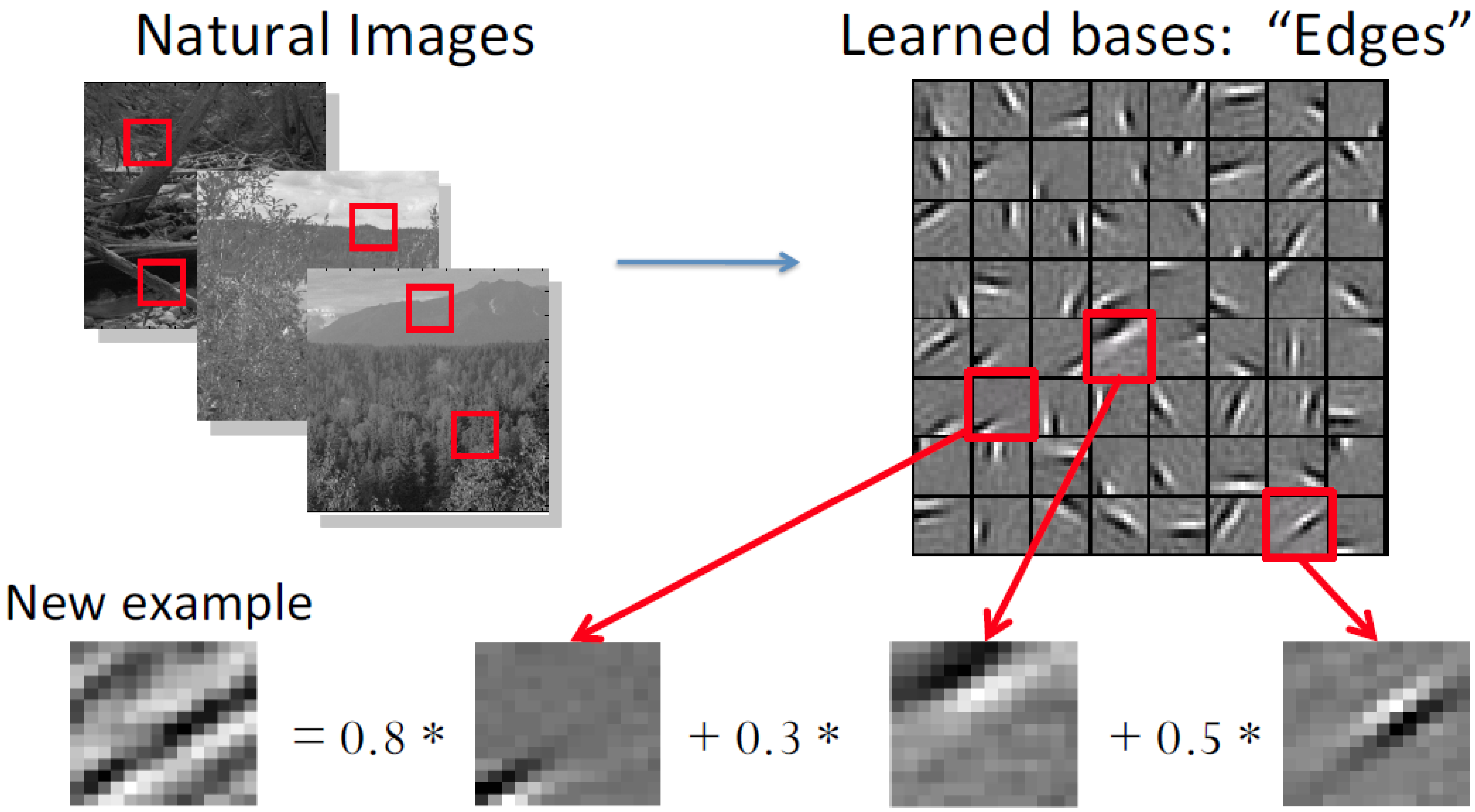
Sparse Coding

- We can also write:

$$\widehat{\mathbf{x}}^{(t)} = \mathbf{D}\,\mathbf{h}(\mathbf{x}^{(t)}) = \sum_{\substack{k \text{ s.t.}\\ h(\mathbf{x}^{(t)})_k \neq 0}} \mathbf{D}_{\cdot,k}\, h(\mathbf{x}^{(t)})_k$$

- D is often referred to as Dictionary
- In certain applications, we know what dictionary matrix to use
- In many cases, we have to learn it

Sparse Coding



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

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

Inference

- Given dictionary D , how do we compute $\mathbf{h}(\mathbf{x}^{(t)})$
- We need to optimize:

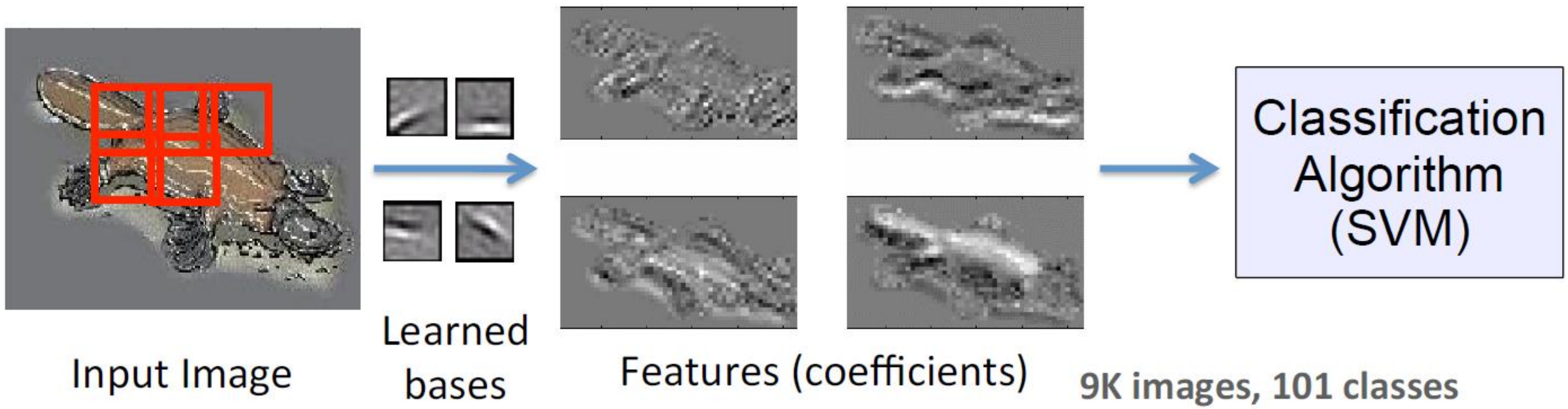
$$l(\mathbf{x}^{(t)}) = \frac{1}{2}||\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}^{(t)}||_2^2 + \lambda||\mathbf{h}^{(t)}||_1$$

- We could use a gradient descent method:

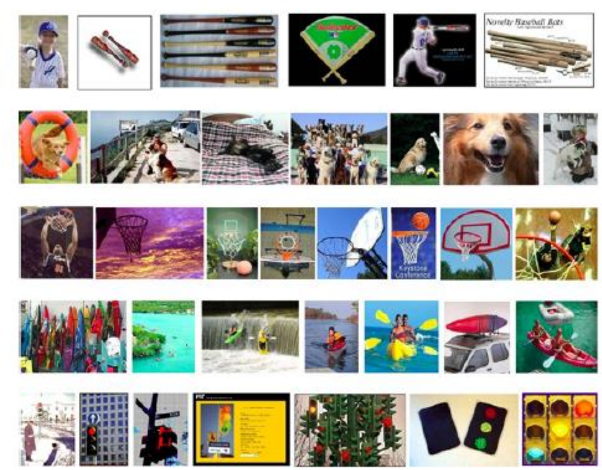
$$\nabla_{\mathbf{h}^{(t)}} l(\mathbf{x}^{(t)}) = \mathbf{D}^\top(\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)}) + \lambda\,\mathrm{sign}(\mathbf{h}^{(t)})$$

Image Classification

- Evaluated on Caltech101 object category dataset



9K images, 101 classes



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

Lee et al., NIPS 2006

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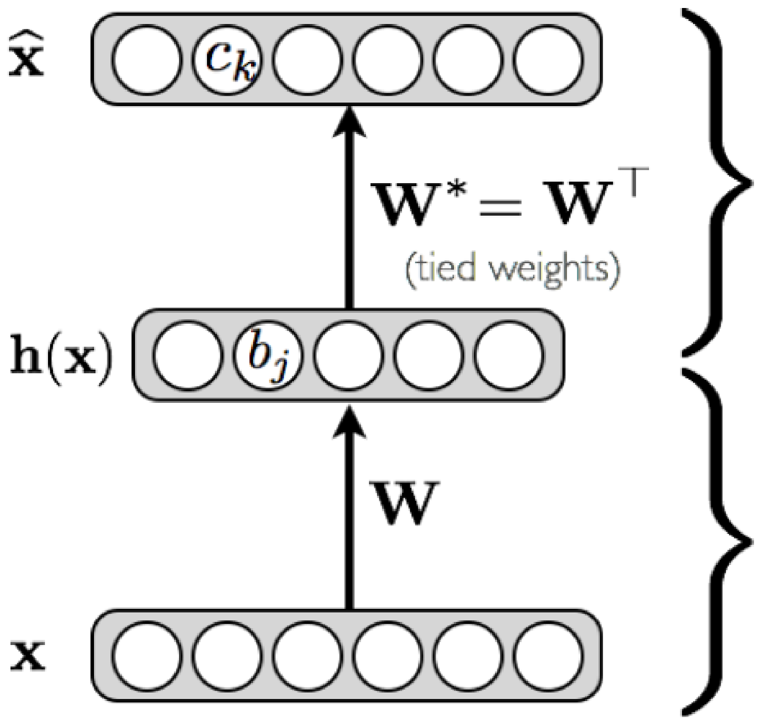
Autoencoder

- Feed-forward neural network trained to reproduce its input at the output layer



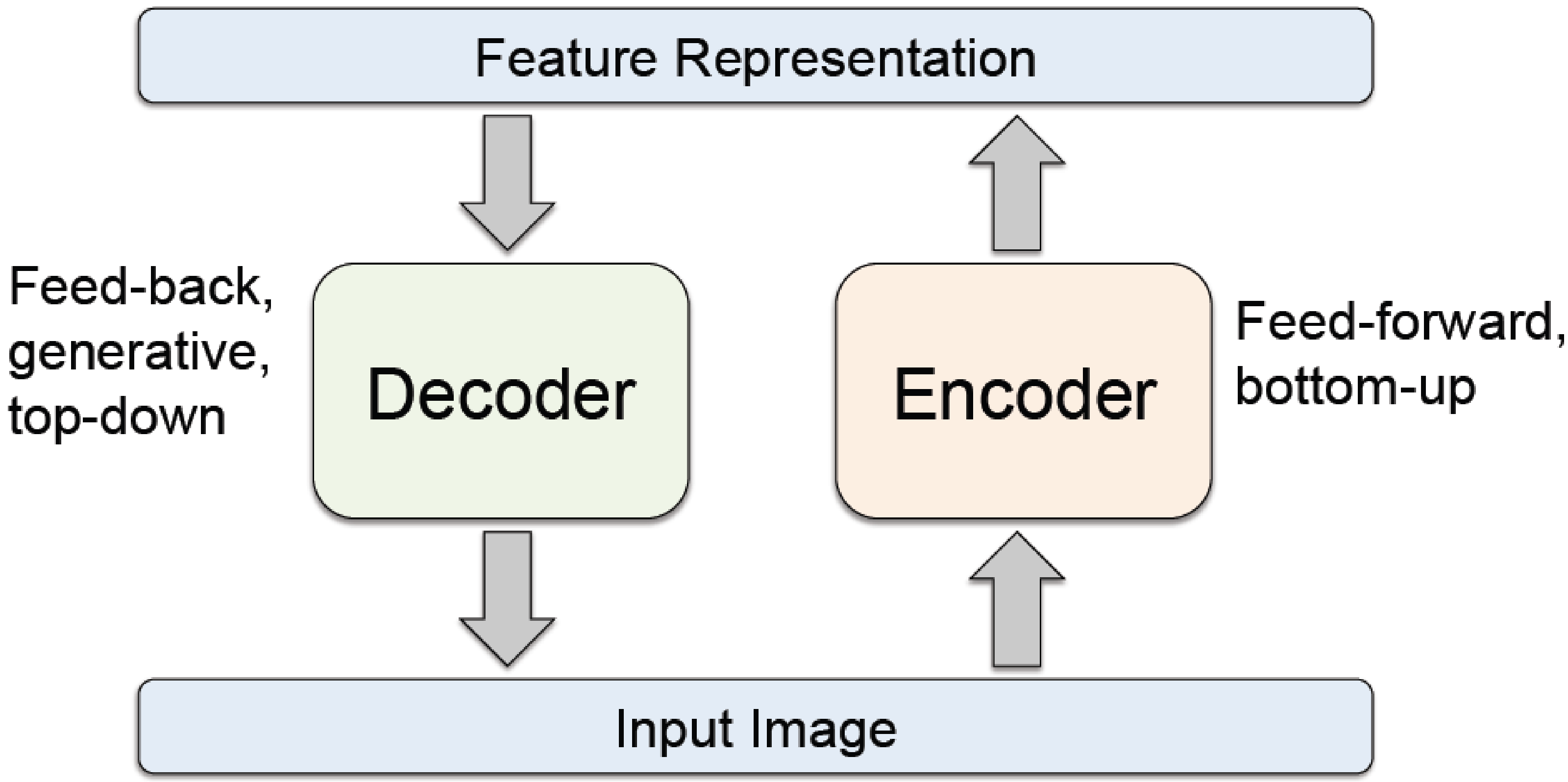
Decoder

$$\begin{aligned}\hat{\mathbf{x}} &= o(\hat{\mathbf{a}}(\mathbf{x})) \\ &= \underbrace{\mathrm{sigm}}_{\text{For binary units}}(\mathbf{c} + \mathbf{W}^* \mathbf{h}(\mathbf{x}))\end{aligned}$$

Encoder

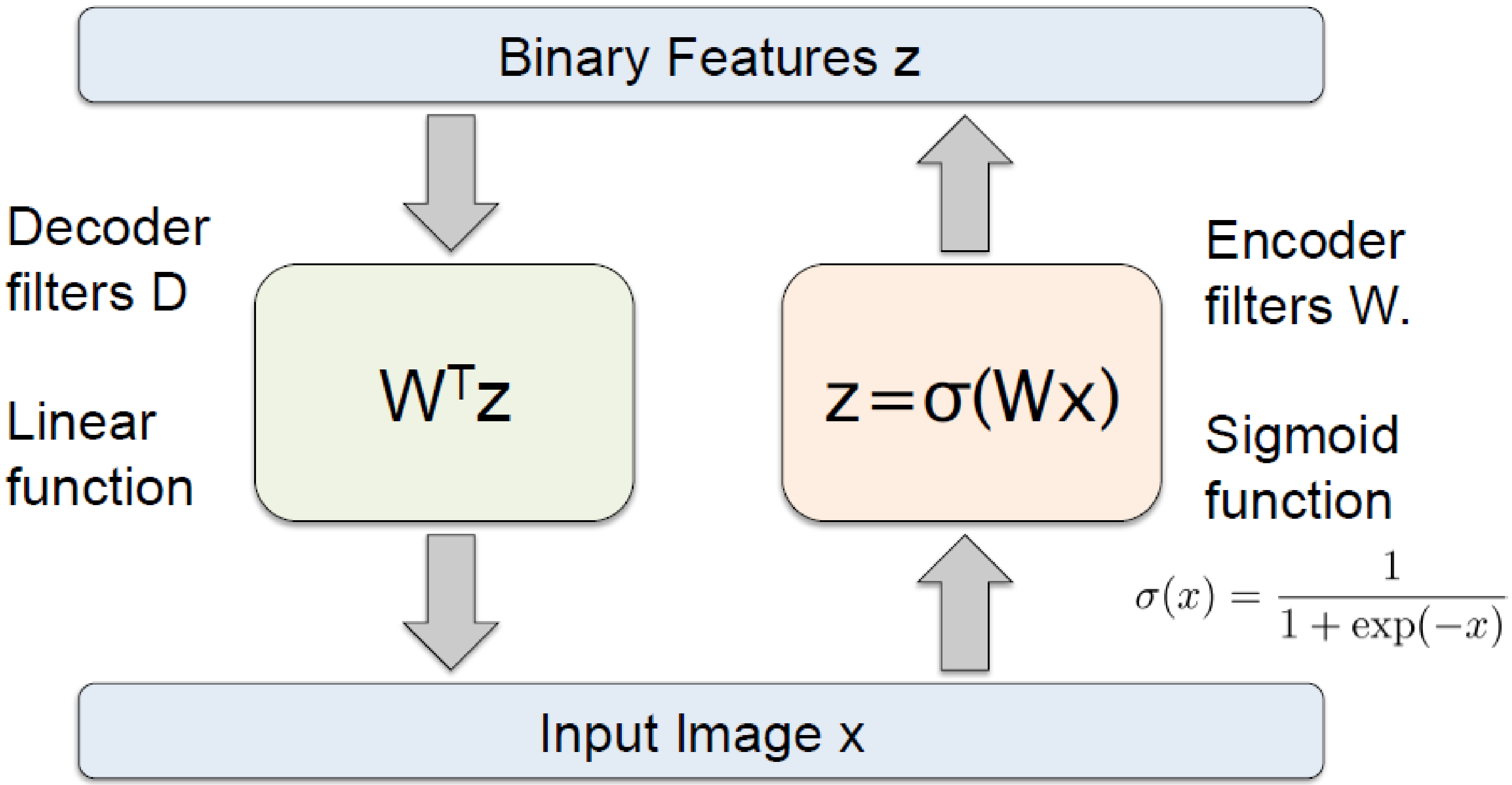
$$\begin{aligned}\mathbf{h}(\mathbf{x}) &= g(\mathbf{a}(\mathbf{x})) \\ &= \mathrm{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})\end{aligned}$$

Autoencoder

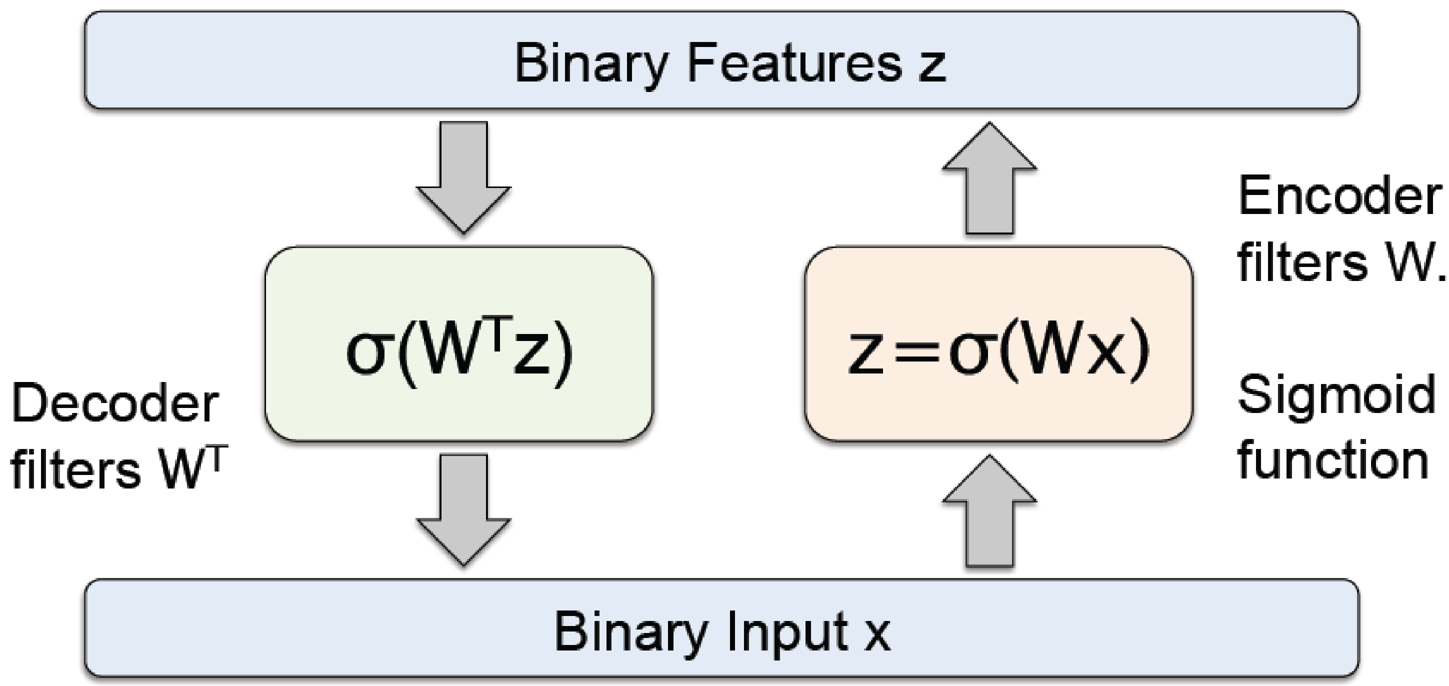


- Details of what goes insider the encoder and decoder matter!
- Need constraints to avoid learning an identity.

Autoencoder



Another Autoencoder Model



- Need additional constraints to avoid learning an identity.
- Relates to Restricted Boltzmann Machines
- Encoder and Decoder filters can be different.

Loss Function

- Loss function for binary inputs

$$l(f(\mathbf{x})) = -\sum_k \left(x_k \log(\widehat{x}_k) + (1 - x_k) \log(1 - \widehat{x}_k)\right)$$

  - Cross-entropy error function (reconstruction loss) $f(\mathbf{x}) \equiv \widehat{\mathbf{x}}$

- Loss function for real-valued inputs

$$l(f(\mathbf{x})) = \frac{1}{2} \sum_k (\widehat{x}_k - x_k)^2$$

  - sum of squared differences (reconstruction loss)
  - we use a linear activation function at the output

Loss Function

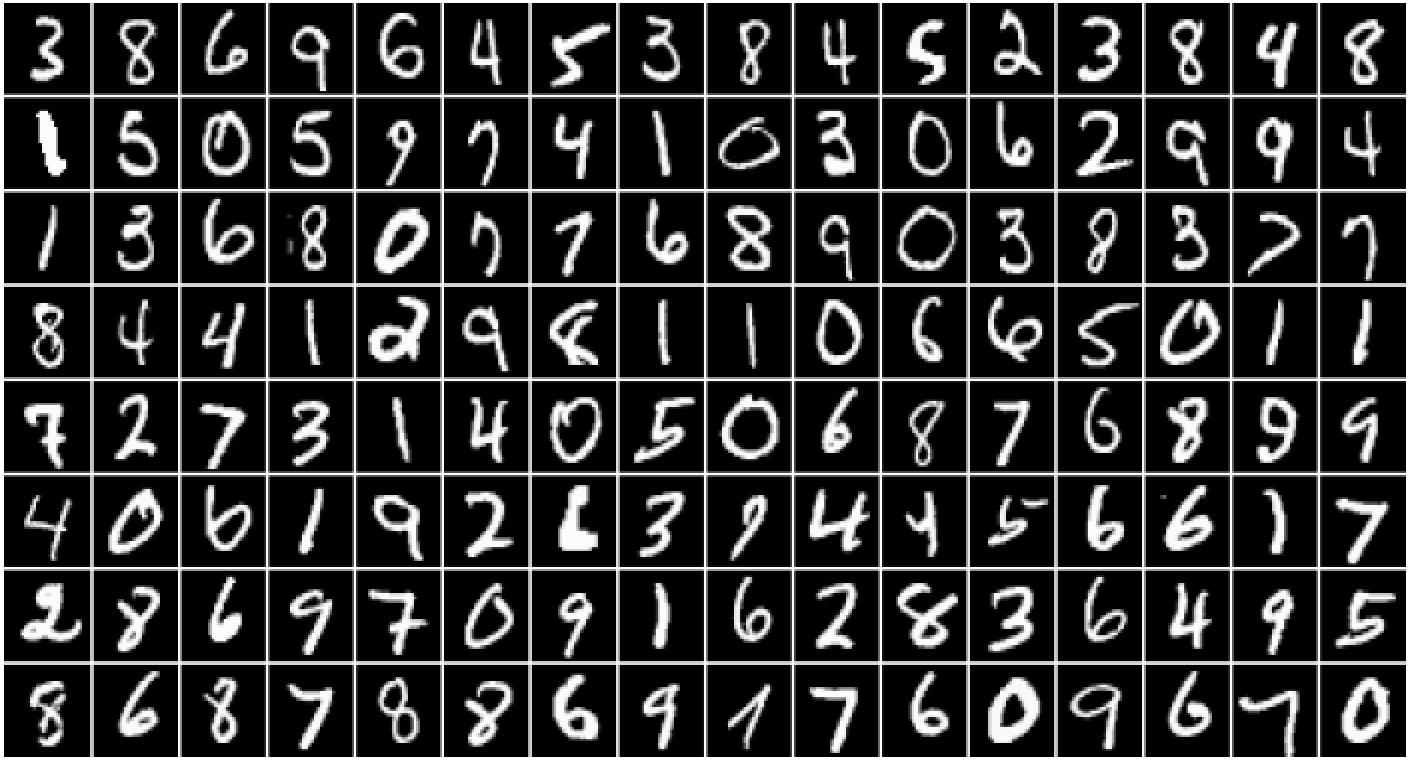
- For both cases, the gradient $\nabla_{\widehat{\mathbf{a}}(\mathbf{x}^{(t)})} l(f(\mathbf{x}^{(t)}))$ has a very simple form:

$$\nabla_{\widehat{\mathbf{a}}(\mathbf{x}^{(t)})} l(f(\mathbf{x}^{(t)})) = \widehat{\mathbf{x}}^{(t)} - \mathbf{x}^{(t)} \qquad f(\mathbf{x}) \equiv \widehat{\mathbf{x}}$$

- Parameter gradients are obtained by backpropagating the gradient $\nabla_{\widehat{\mathbf{a}}(\mathbf{x}^{(t)})} l(f(\mathbf{x}^{(t)}))$ like in a regular network
  - important: when using tied weights ($\mathbf{W}^* = \mathbf{W}^\top$), $\nabla_{\mathbf{W}} l(f(\mathbf{x}^{(t)}))$ is the sum of two gradients
  - this is because $\mathbf{W}$ is present in the encoder and in the decoder

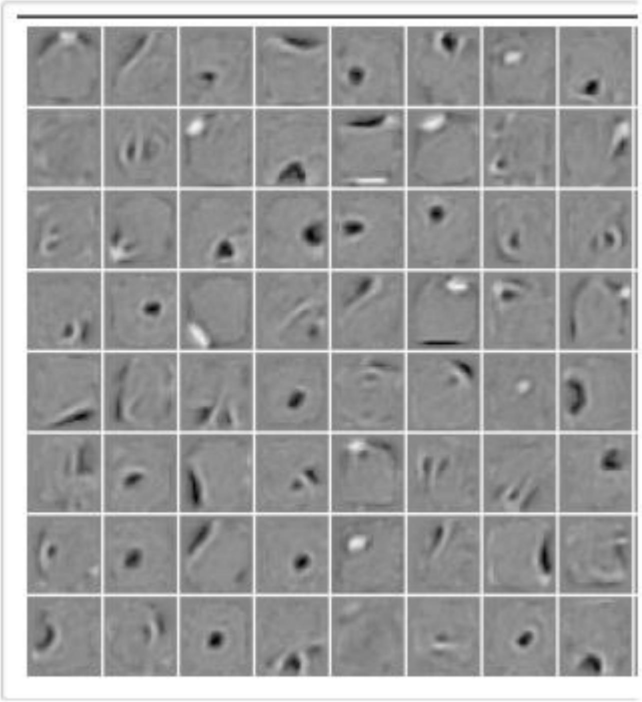
Example: MNIST

- MNIST dataset:

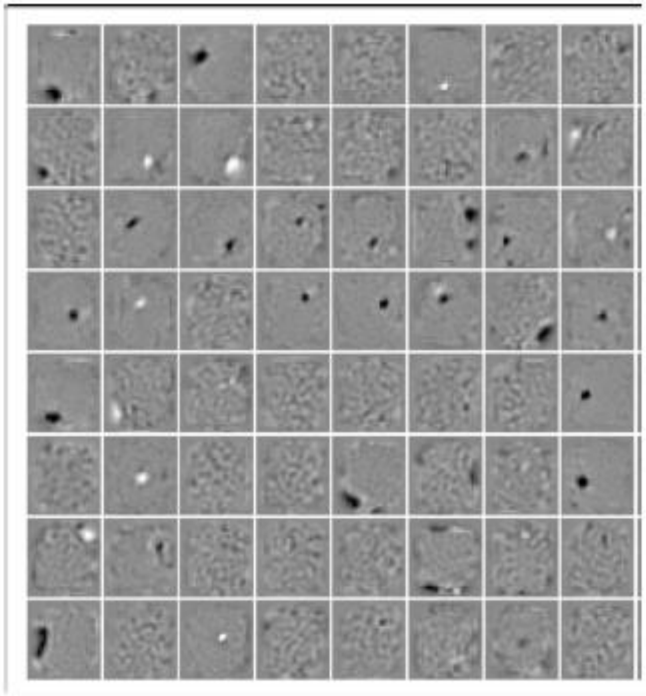


Learned Features

- MNIST dataset:

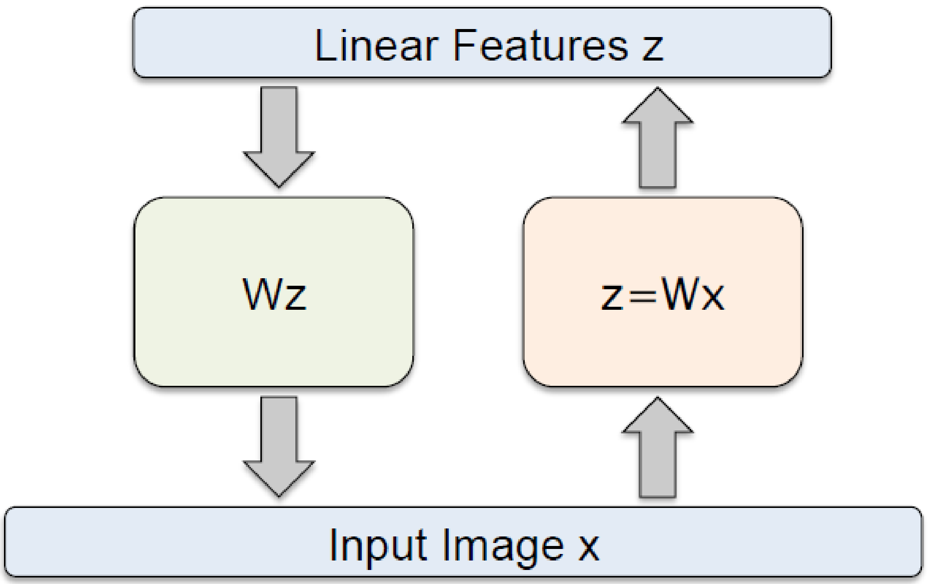


RBM



Autoenncoder

Linear Autoencoder & PCA



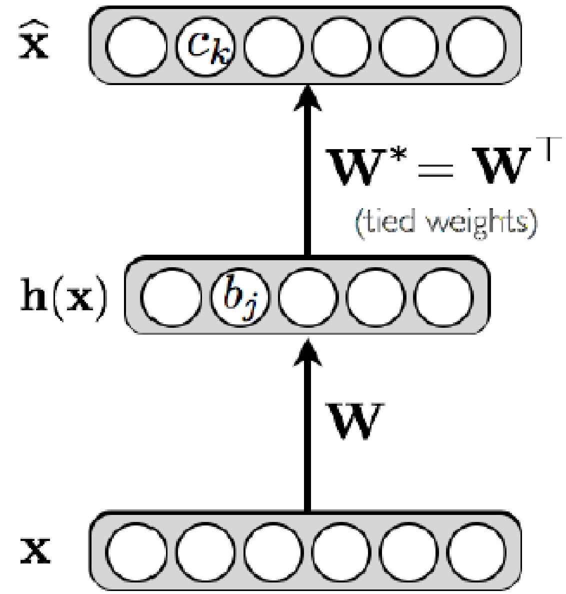
- If the hidden and output layers are linear, it will learn hidden units that are a linear function of the data and minimize the squared error.

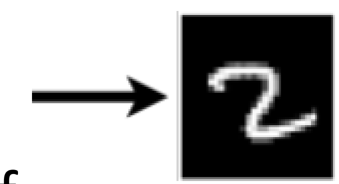
- The K hidden units will span the same space as the first k principal components. The weight vectors may not be orthogonal.

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

Undercomplete Representation

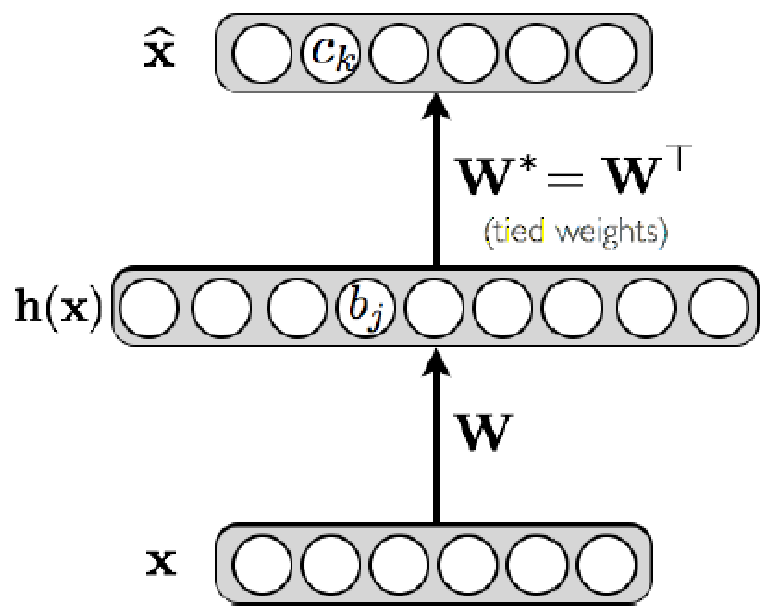
- Hidden layer is undercomplete if smaller than the input layer (bottleneck layer, e.g. dimensionality reduction):
  - hidden layer ''compresses'' the input
  - will compress well only for the training distribution
- Hidden units will be
  - good features for the training distribution
  - will not be robust to other types of input





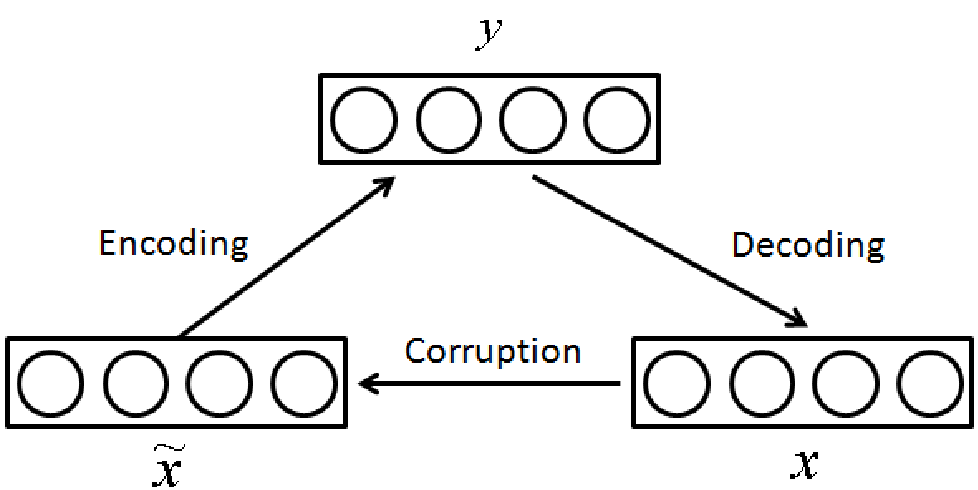
Overcomplete Representation

- Hidden layer is overcomplete if greater than the input layer
  - no compression in hidden layer
  - each hidden unit could copy a different input component
- No guarantee that the hidden units will extract meaningful structure



Denoising Autoencoder

- To force the hidden layer to discover more robust features, train the autoencoder to reconstruct the input from a corrupted version of it
  - Randomly set some of the inputs (as many as half of them) to 0.
  - Predict the corrupted (i.e. missing) values from the uncorrupted (i.e., non-missing) values.
  - The input can be corrupted in other ways.

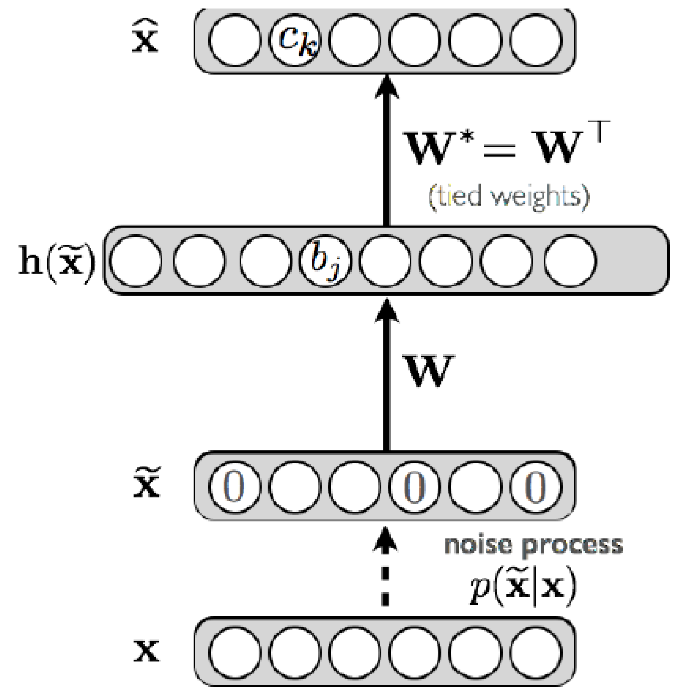


Denoising Autoencoder

- Idea: representation should be robust to introduction of noise:
  - random assignment of subset of inputs to 0, with probability
  - Similar to dropouts on the input layer
  - Gaussian additive noise

- Reconstruction $\widehat{\mathbf{x}}$ computed from the corrupted input $\widetilde{\mathbf{x}}$

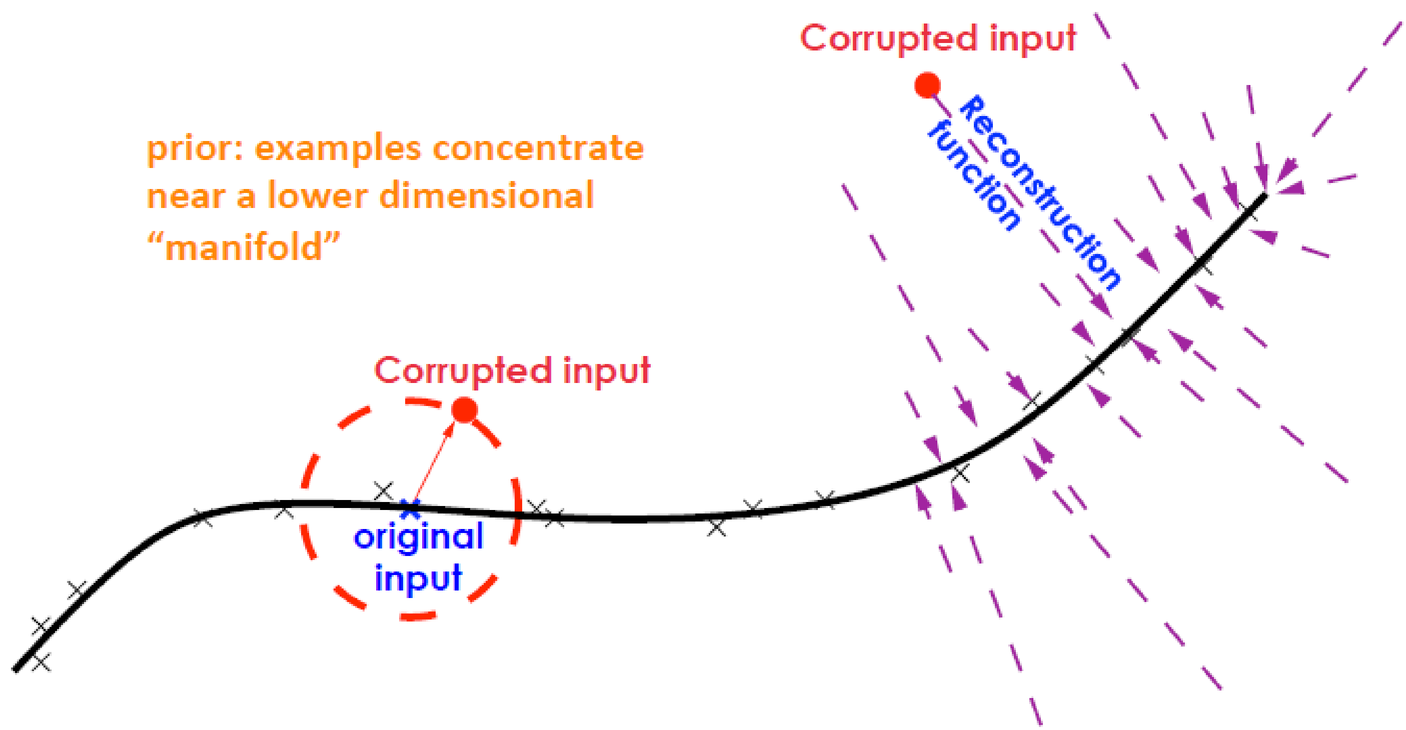
- Loss function compares $\widehat{\mathbf{x}}$ reconstruction with the noiseless input $\mathbf{x}$



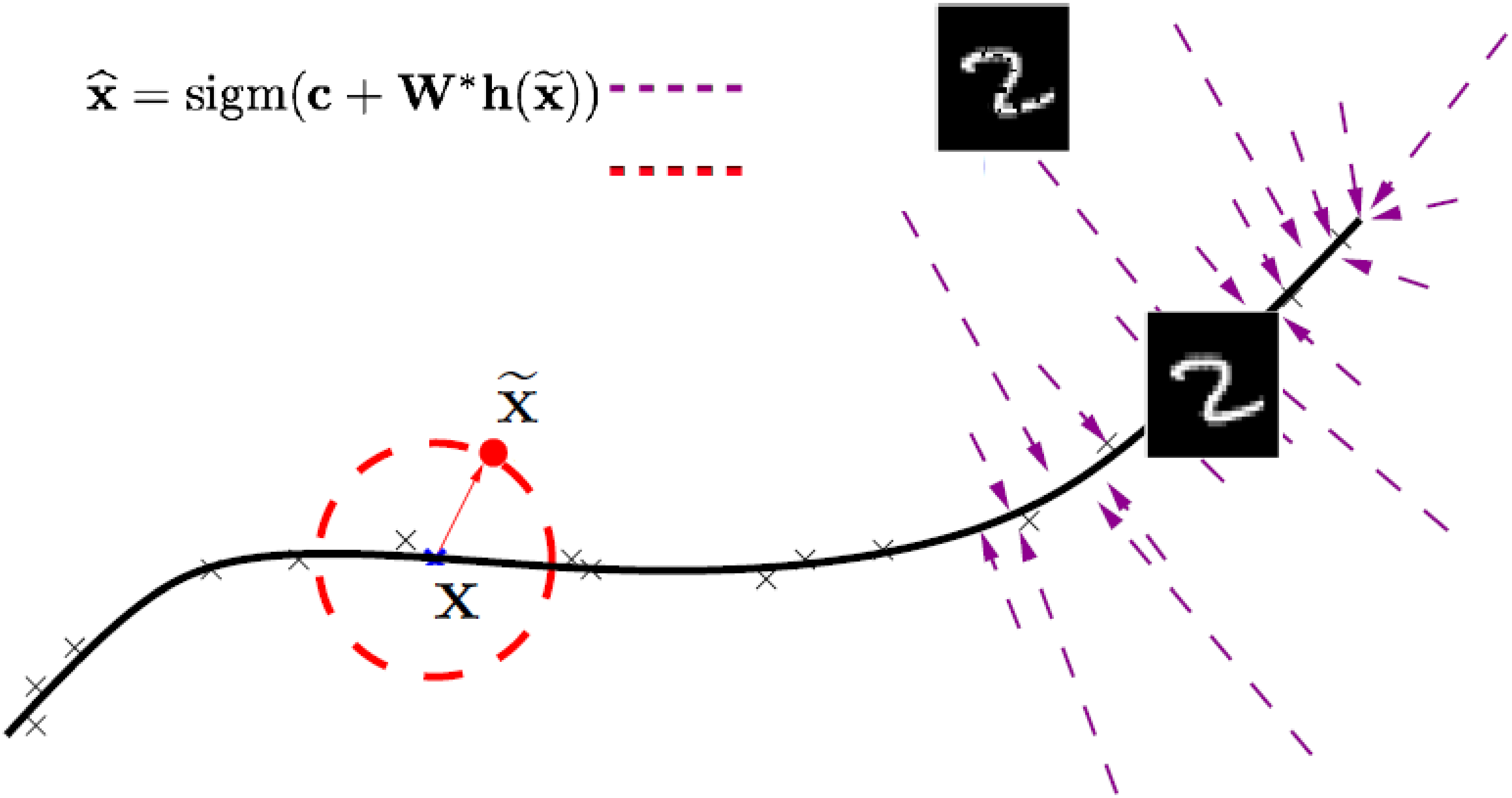
(Vincent et.al., ICML 2008)

Denoising Autoencoder

- The learner must capture the structure of the input distribution in order to optimally undo the effect of the corruption process
- The denoising autoencoder is learning a reconstruction function that corresponds to a vector field pointing towards high-density regions (the manifold where examples concentrate)

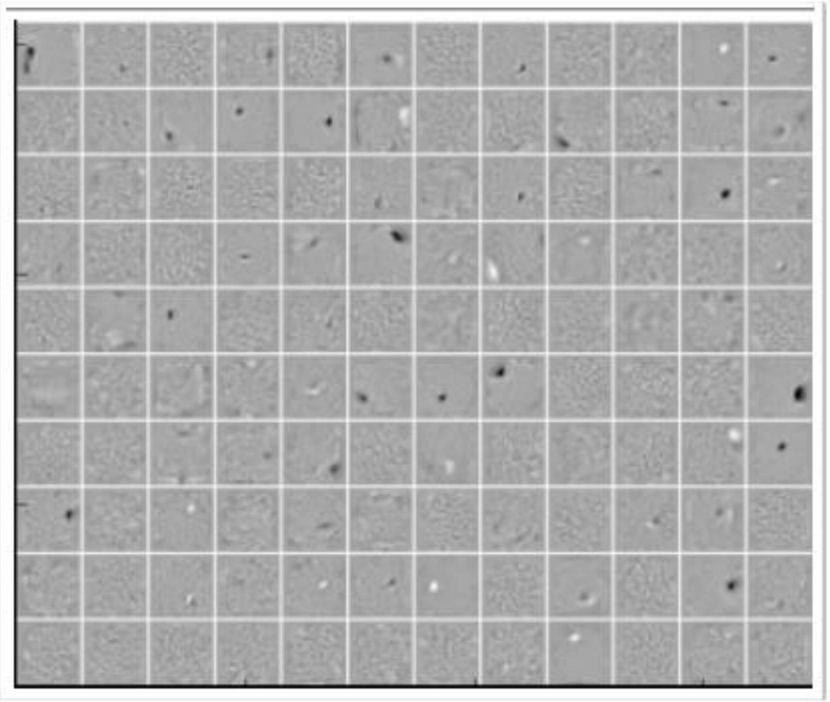


Denoising Autoencoder

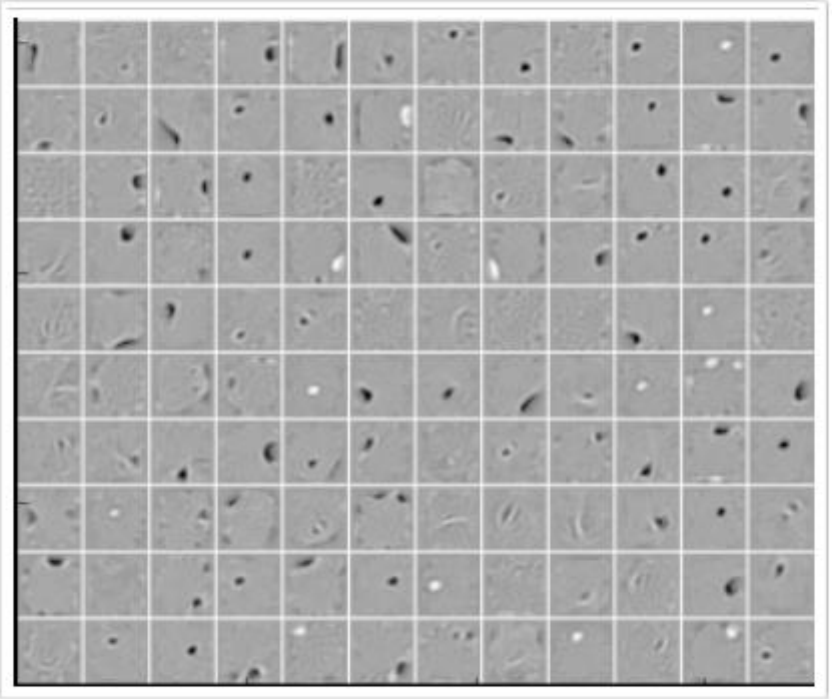


Learned Filters

Non-corrupted

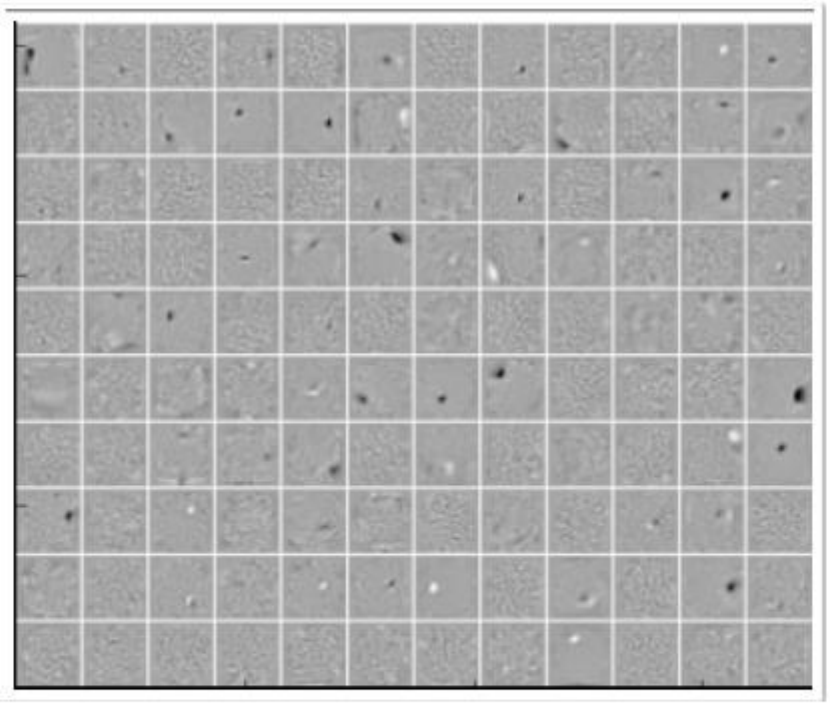


25% corrupted input

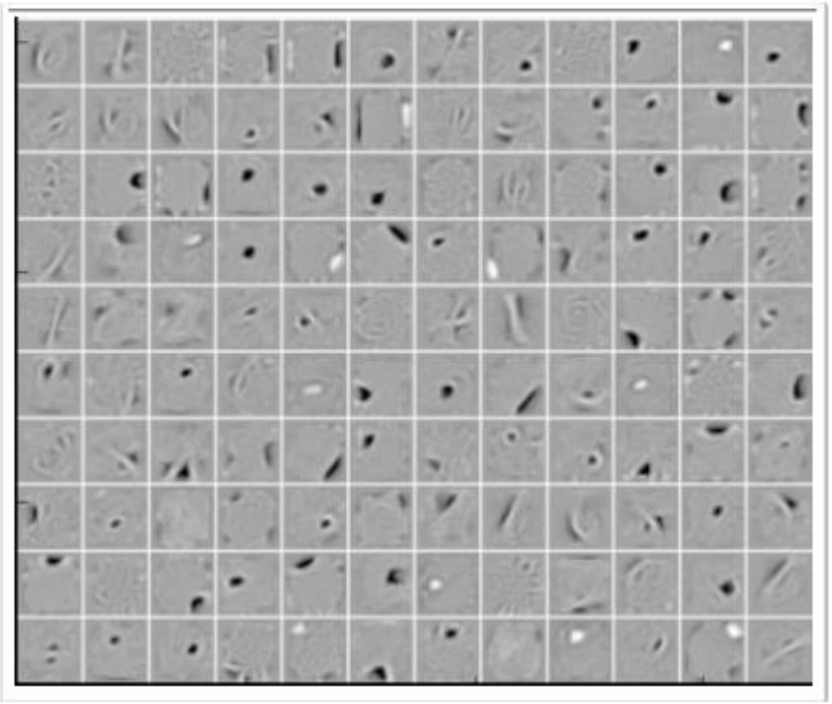


Learned Filters

Non-corrupted

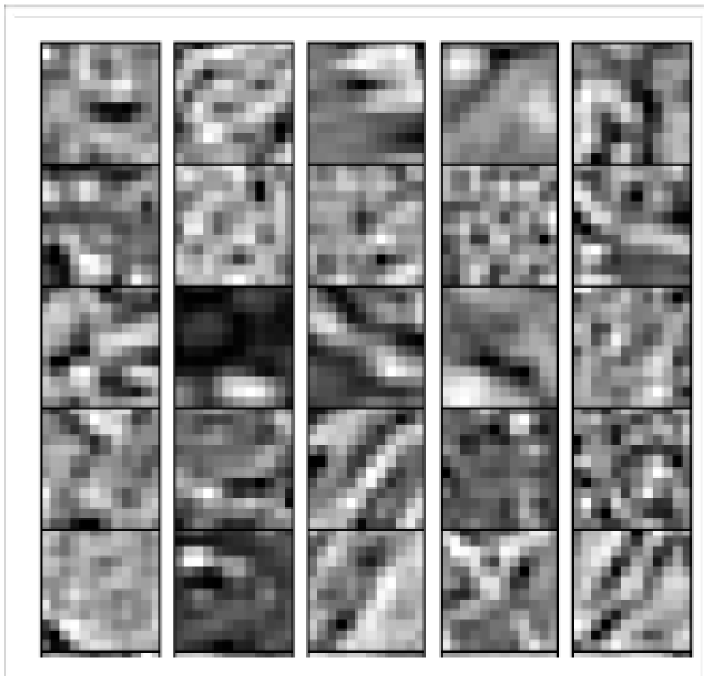


50% corrupted input

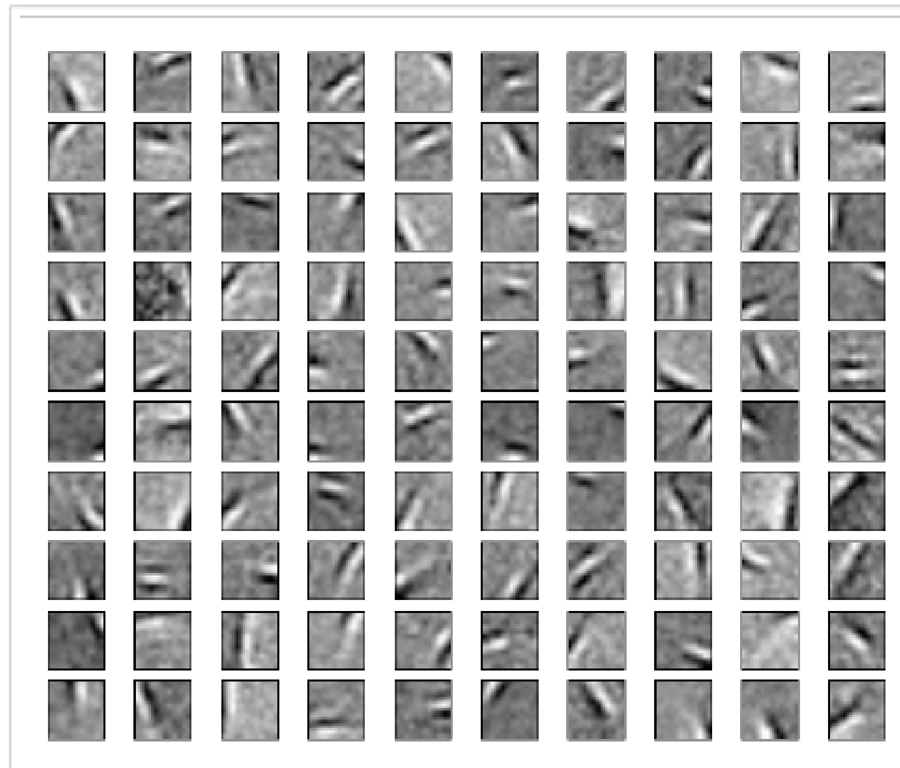


Squared Error Loss

- Training on natural image patches, with squared loss



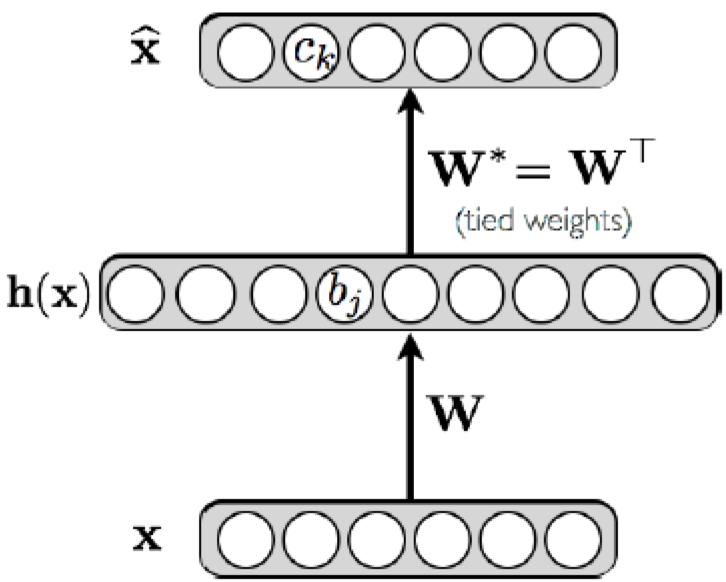
Data



Filters

Contractive Autoencoder

- Alternative approach to avoid uninteresting solutions
  - add an explicit term in the loss that penalizes that solution
- We wish to extract features that only reflect variations observed in the training set
  - we'd like to be invariant to the other variations



Contractive Autoencoder

- Consider the following loss function:

$$\underbrace{l(f(\mathbf{x}^{(t)}))}_{\text{Reconstruction Loss}} + \lambda \underbrace{||\nabla_{\mathbf{x}^{(t)}} \mathbf{h}(\mathbf{x}^{(t)})||_F^2}_{\text{Jacobian of Encoder}}$$

- For the binary observations:

$$l(f(\mathbf{x}^{(t)})) = -\sum_k \left(x_k^{(t)} \log(\widehat{x}_k^{(t)}) + (1 - x_k^{(t)}) \log(1 - \widehat{x}_k^{(t)}) \right)$$

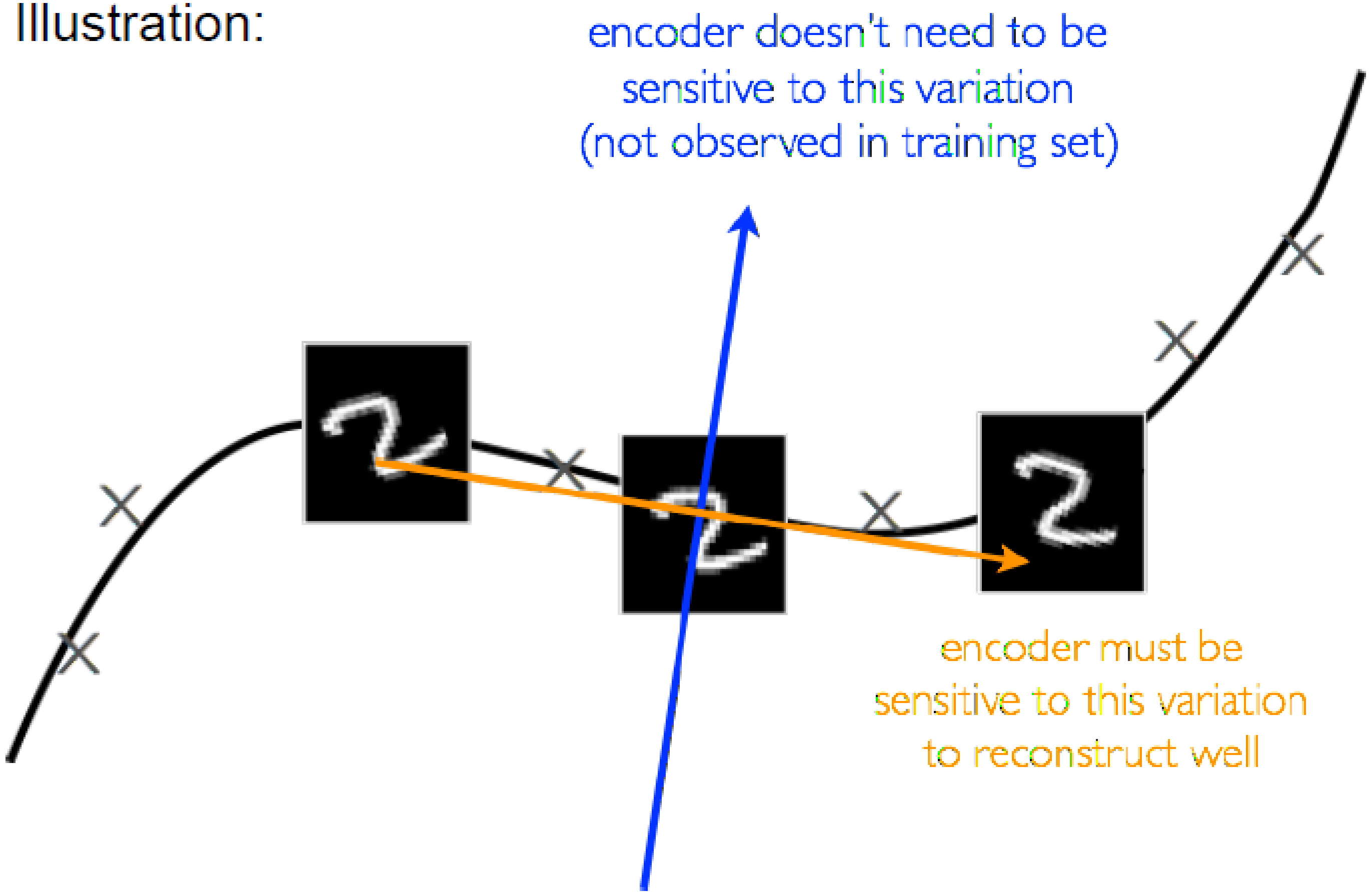
Autoencoder attempts to preserve all information

$$||\nabla_{\mathbf{x}^{(t)}} \mathbf{h}(\mathbf{x}^{(t)})||_F^2 = \sum_j \sum_k \left(\frac{\partial h(\mathbf{x}^{(t)})_j}{\partial x_k^{(t)}} \right)^2$$

Encoder throws away all information

Contractive Autoencoder

- Illustration:



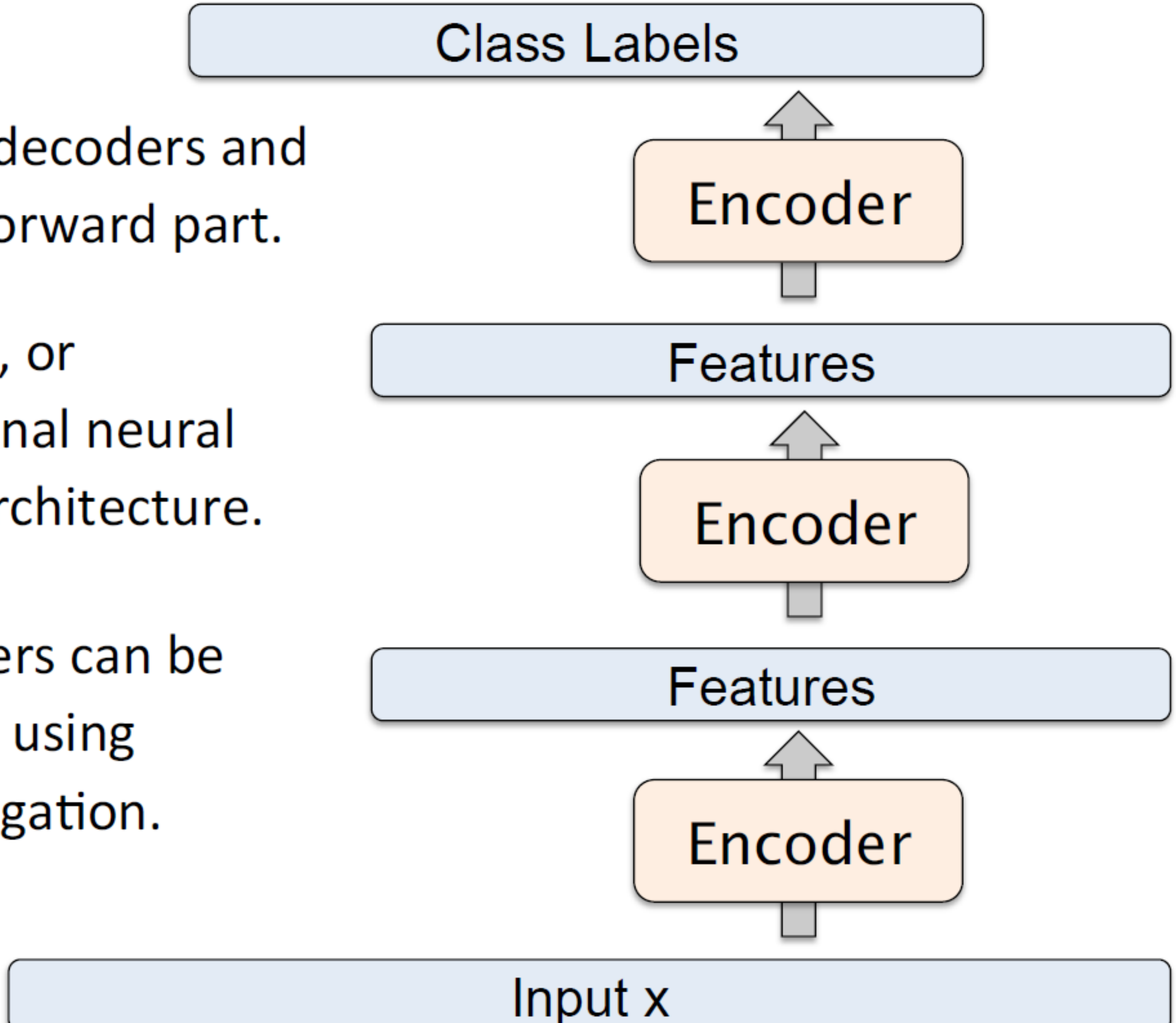
Pros and Cons

- Advantage of denoising autoencoder: simpler to implement
  - requires adding one or two lines of code to regular autoencoder
  - no need to compute Jacobian of hidden layer

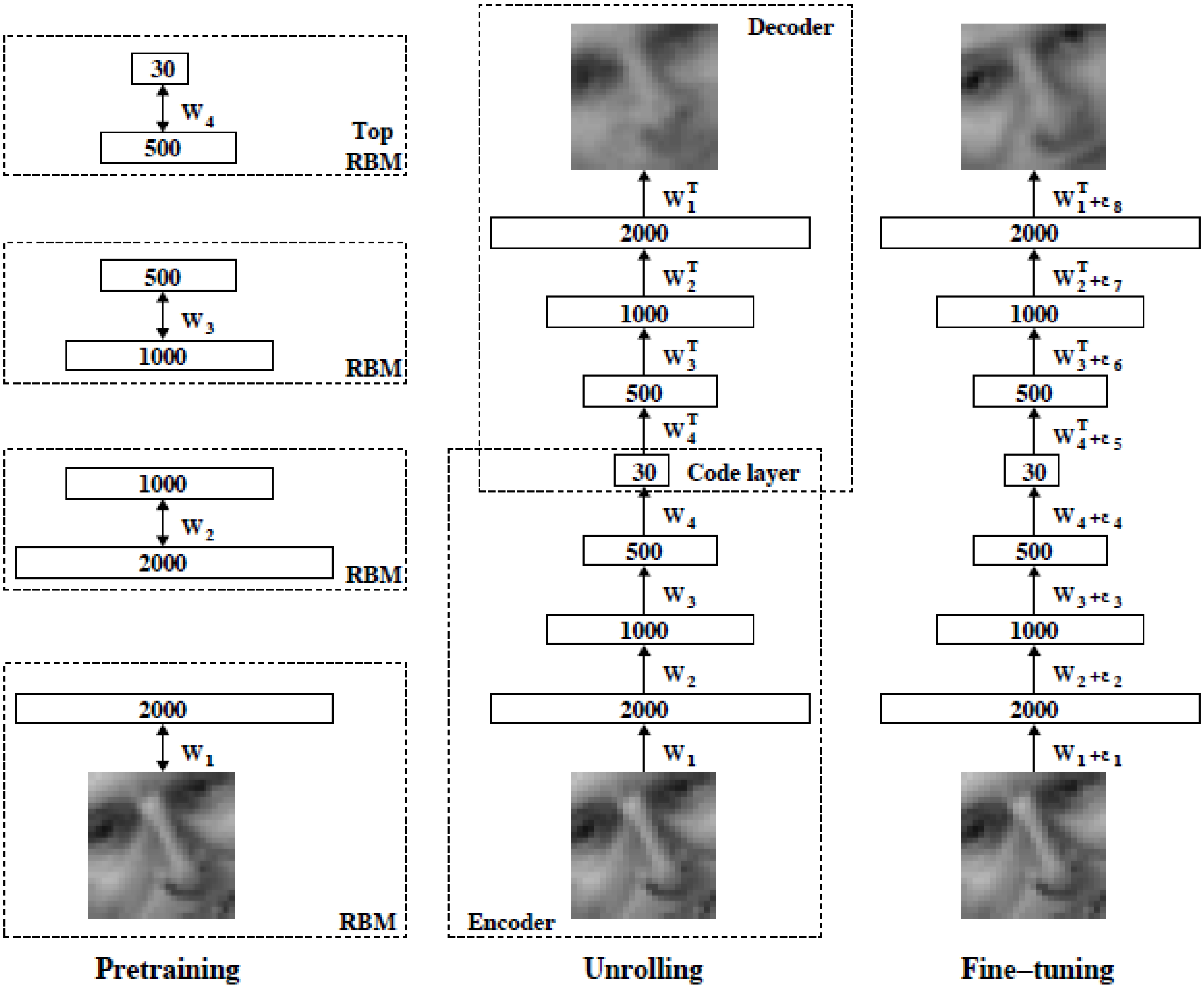
- Advantage of contractive autoencoder: gradient is deterministic
  - can use second order optimizers (conjugate gradient, LBFGS, etc.)
  - might be more stable than denoising autoencoder, which uses a sampled gradient

Stacked Autoencoder

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



Deep Autoencoder



Deep Autoencoder

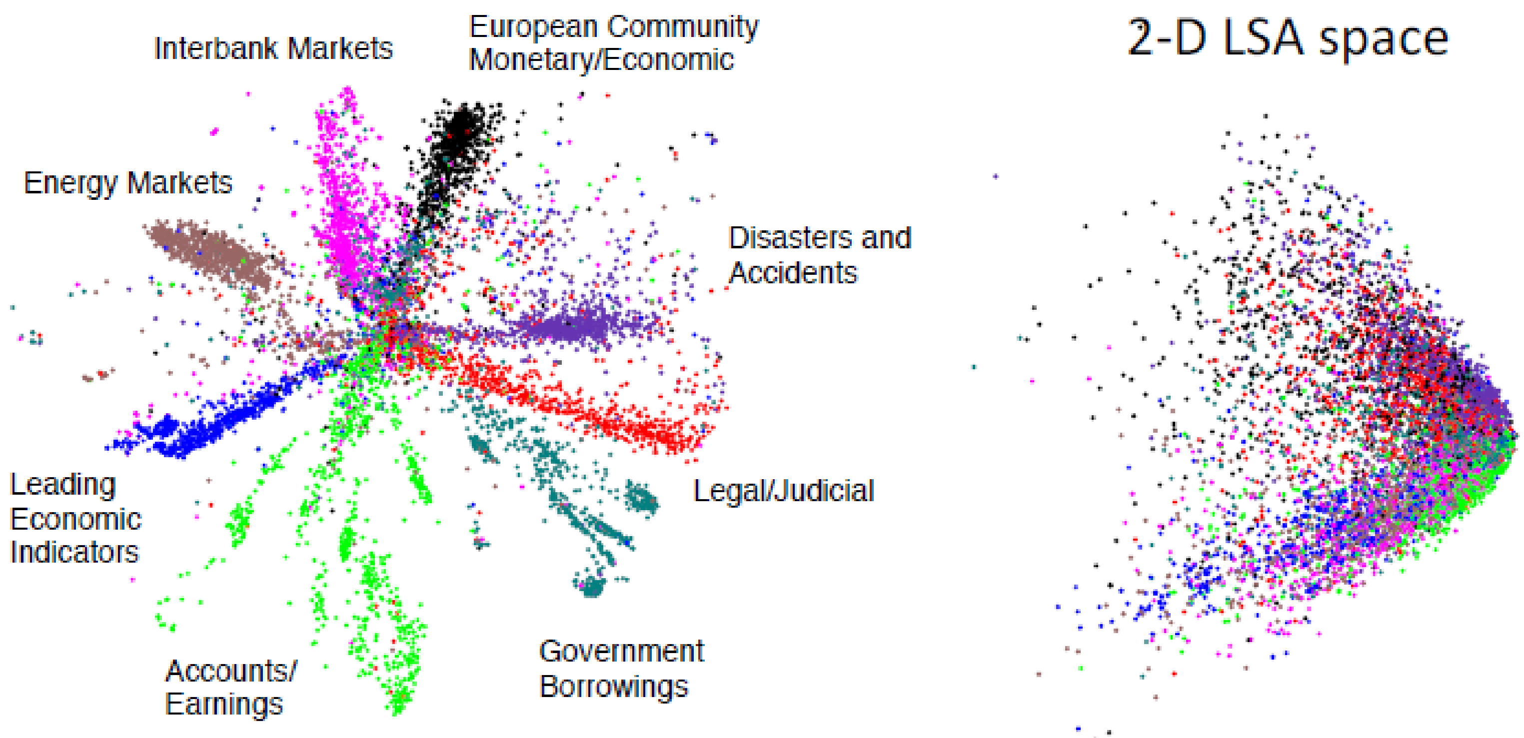
- We used 25x25 – 2000 – 1000 – 500 – 30 autoencoder to extract 30-D real-valued codes for Olivetti face patches.

- **Top**: Random samples from the test dataset.
- **Middle**: Reconstructions by the 30-dimensional deep autoencoder.
- **Bottom**: Reconstructions by the 30-dimensional PCA

Deep Autoencoder

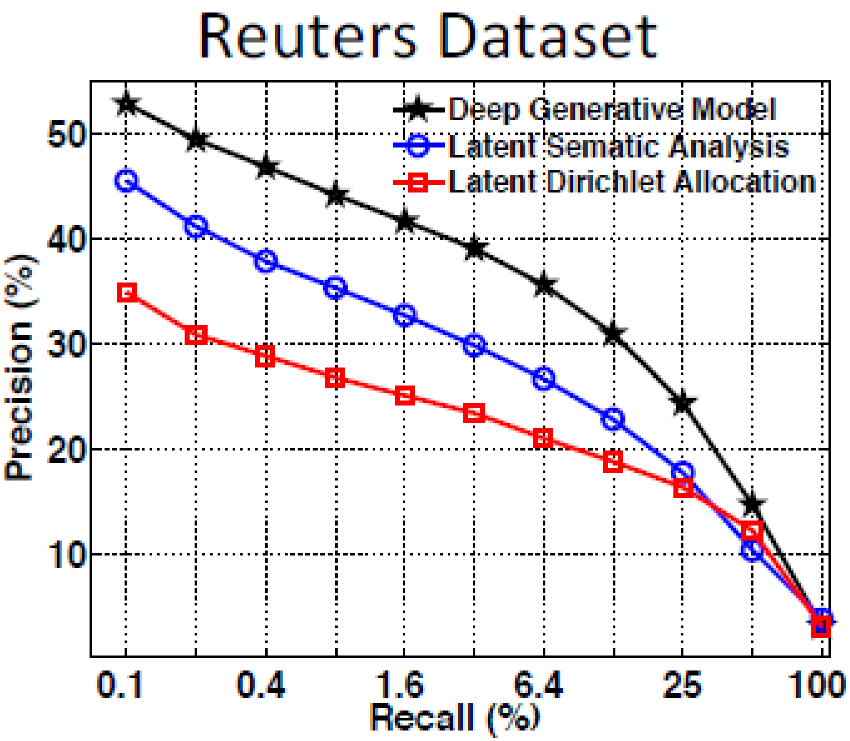
- Very difficult to optimize deep autoencoders using backpropagation
- Pre-training + fine-tuning
  - First train a stack of RBMs
  - Then "unroll" them
  - Then fine-tune with backpropagation

Information Retrieval



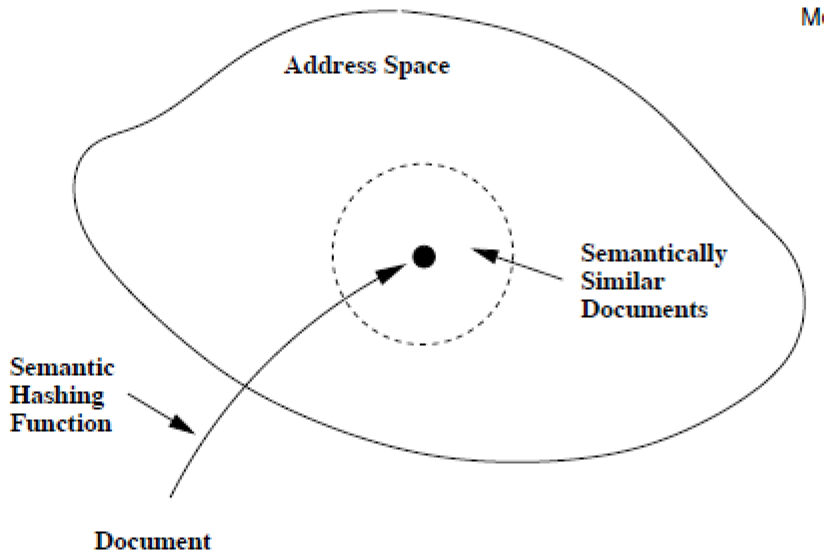
- The Reuters Corpus Volume II contains 804,414 newswire stories (randomly split into **402,207 training and 402,207 test).**
- “Bag-of-words” representation: each article is represented as a vector containing the counts of the most frequently used 2000 words in the training set.

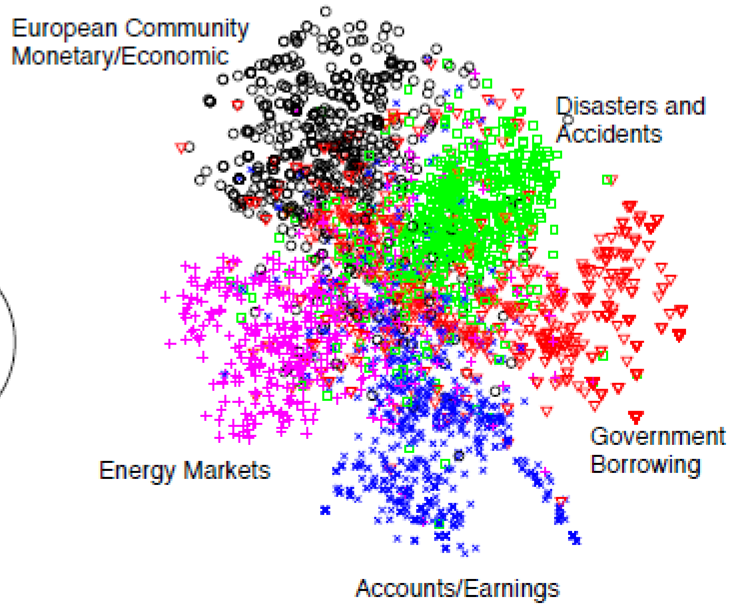
Information Retrieval



- Reuters dataset: 804,414 newswire stories.
- Deep generative model significantly outperforms LSA and LDA topic models

Semantic Hashing

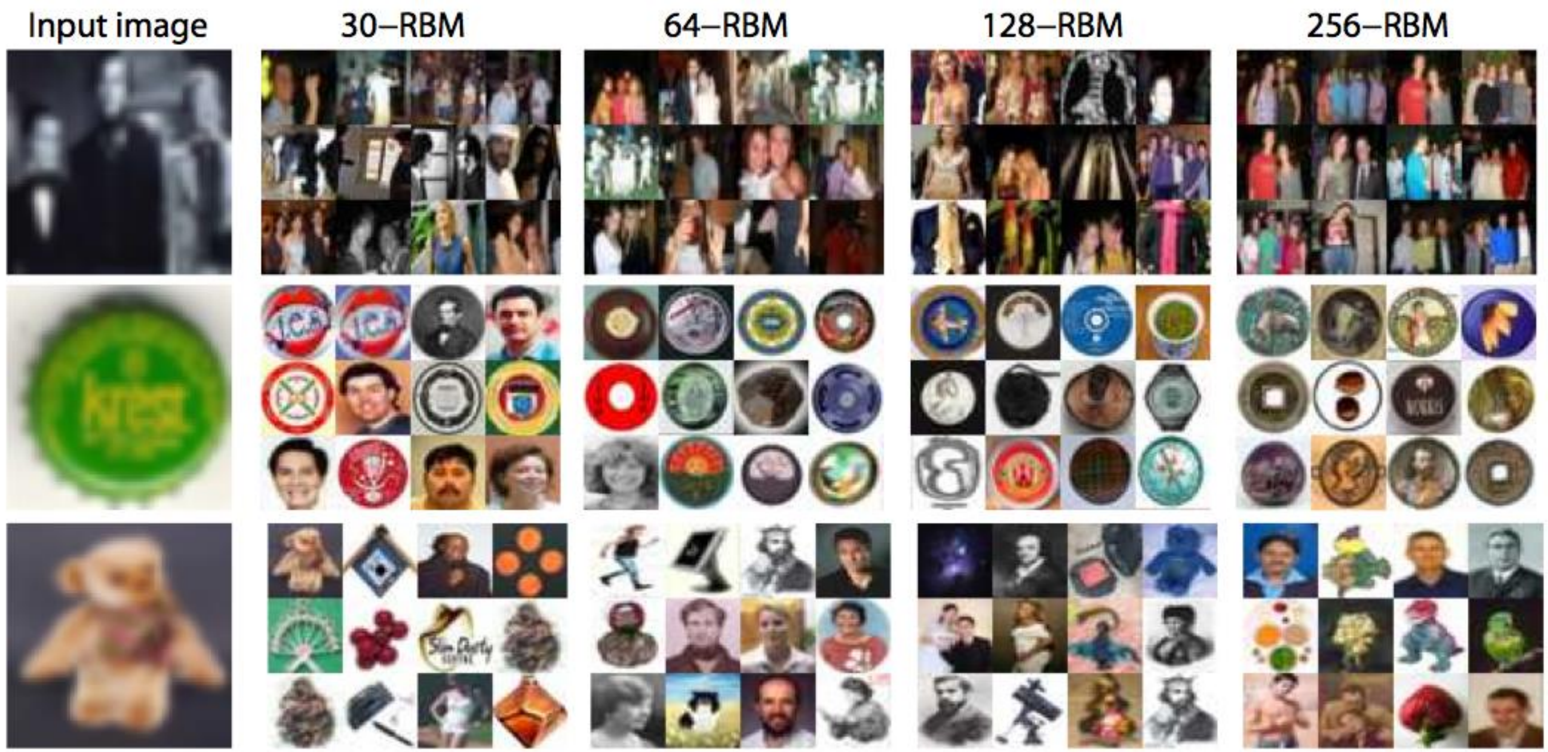




- Learn to map documents into **semantic 20-D binary codes.**
- Retrieve similar documents stored at the nearby addresses **with no search at all.**

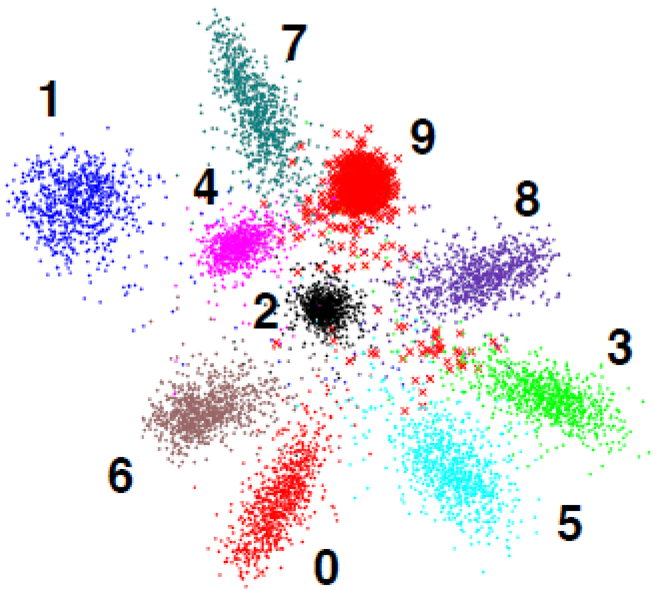
Searching Image Database using Binary Codes

- Map images into binary codes for fast retrieval



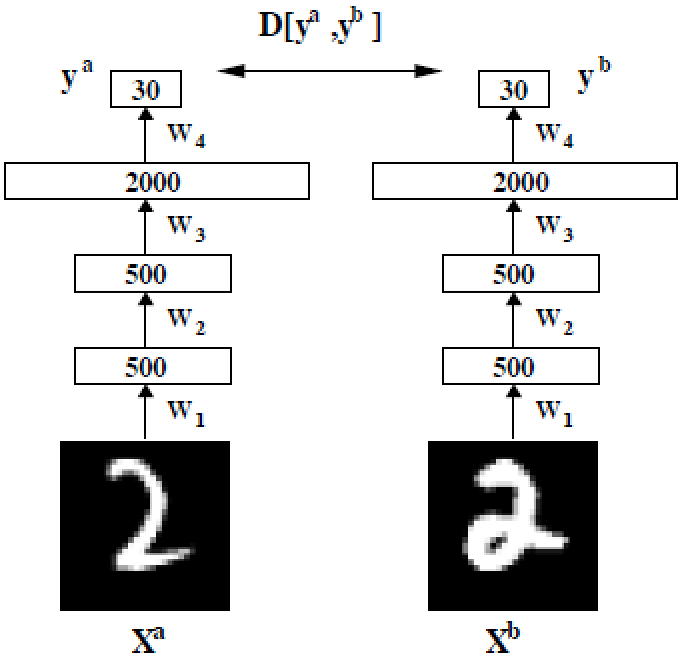
- Small Codes, Torralba, Fergus, Weiss, CVPR 2008
- Spectral Hashing, Y. Weiss, A. Torralba, R. Fergus, NIPS 2008
- Kulis and Darrell, NIPS 2009, Gong and Lazebnik, CVPR 20111
- Norouzi and Fleet, ICML 2011,

Learning Similarity Measures



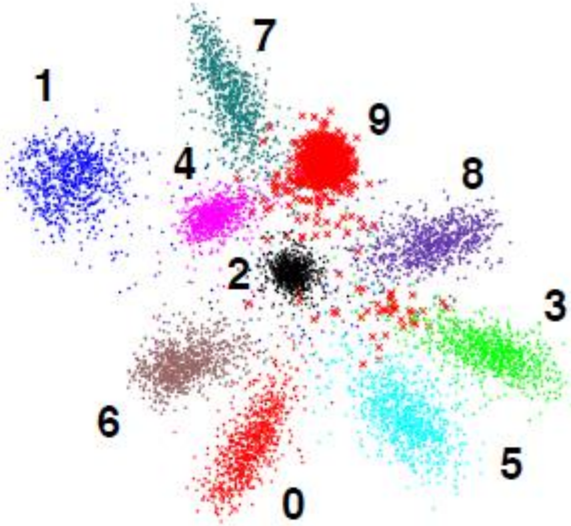
Related to Siamese Networks of LeCun.

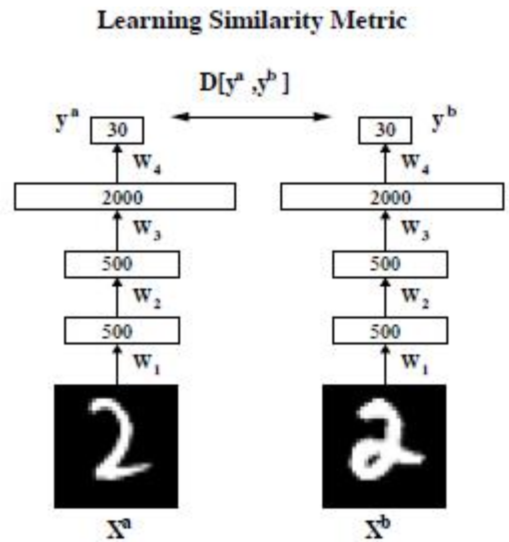
Maximize the Agreement



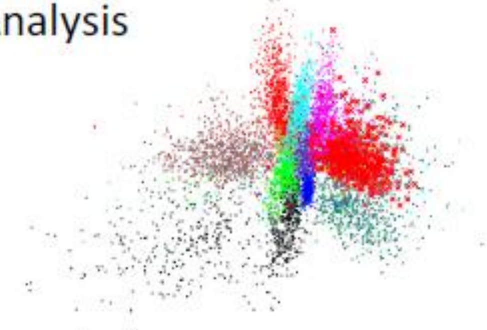
- Learn a nonlinear transformation of the input space.
- Optimize to make KNN perform well in the low-dimensional feature space

Learning Similarity Measures

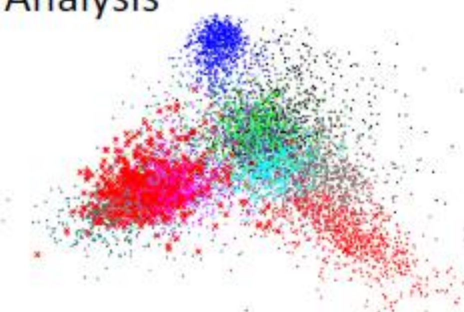




Neighborhood Component Analysis



Linear discriminant Analysis



PCA

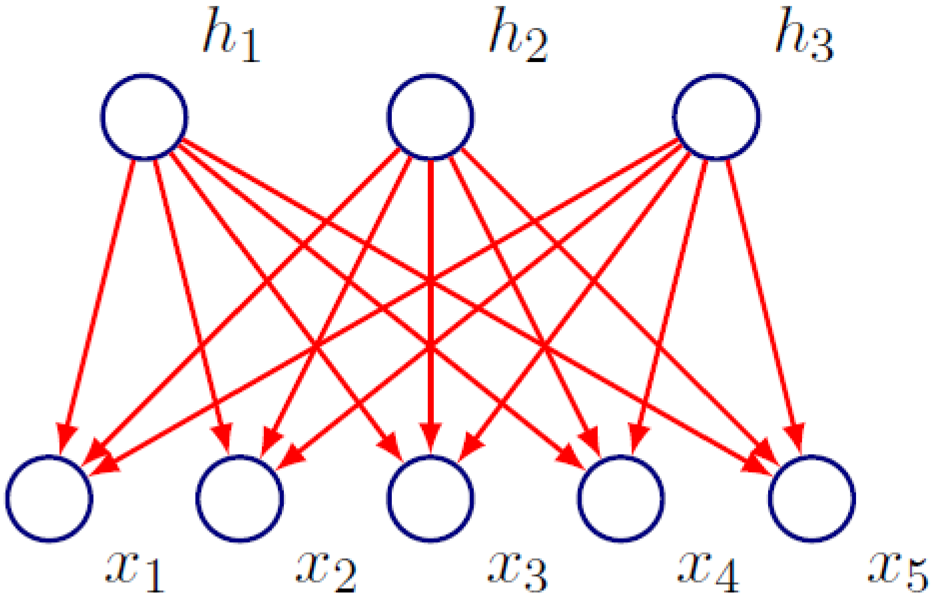
Outline

1. Course Review
2. Linear Factor Model
3. Autoencoder
4. DBN and RBM

More General Models

- Suppose P(h) can not be assumed to have a nice Gaussian form
- The decoding of the input from the latent states can be a complicated non-linear function
- Estimation and inference can get complicated!

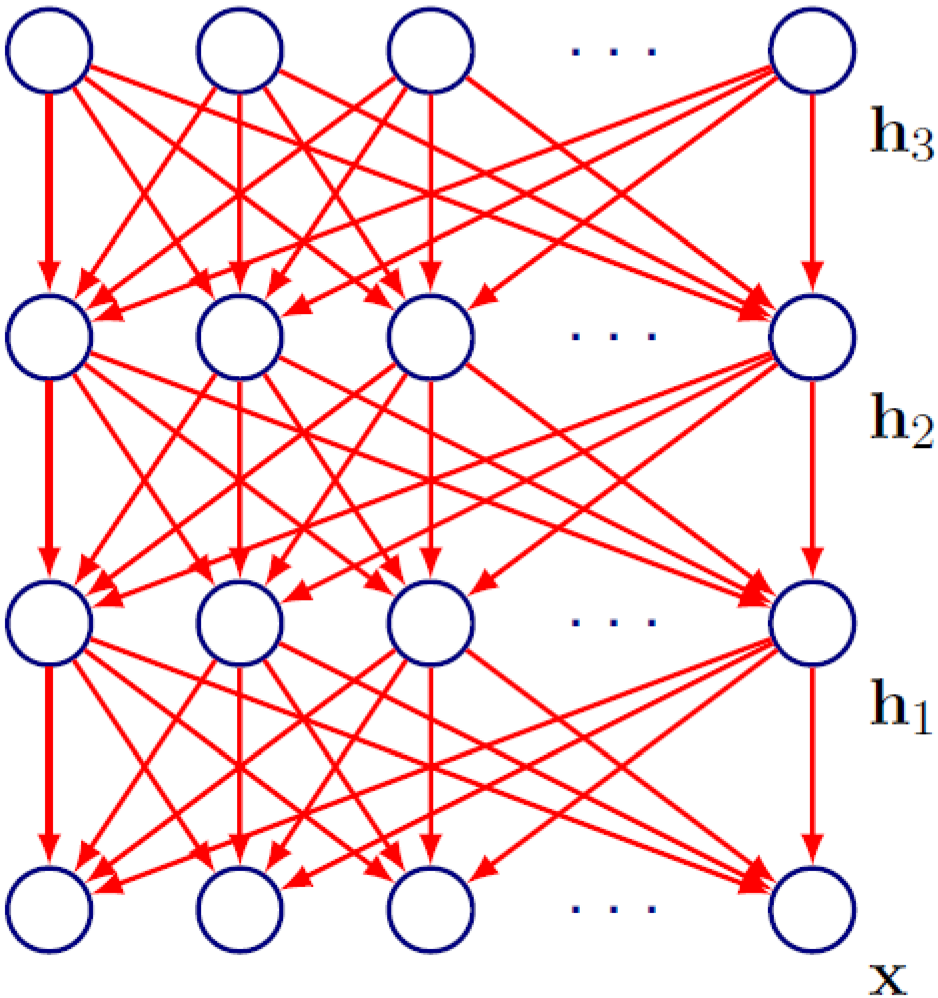
Earlier we had:



Quick Review

- Generative models can be modeled as directed graphical models
- The nodes represent random variables and arcs indicate dependency
- Some of the random variables are observed, others are hidden

Sigmoid Belief Networks



- Just like a feedfoward network, but with arrows reversed.

Sigmoid Belief Networks

- Let x = h^0. Consider binary activations, then:

$$P(\mathbf{h}_i^k = 1 | \mathbf{h}^{k+1}) = sigm(b_i^k + \sum_j W_{i,j}^{k+1} \mathbf{h}_j^{k+1})$$

- The joint probability factorizes as:

$$P(\mathbf{x}, \mathbf{h}^1, \ldots, \mathbf{h}^l) = P(\mathbf{h}^l) \left(\prod_{k=1}^{l-1} P(\mathbf{h}^k | \mathbf{h}^{k+1}) \right) P(\mathbf{x} | \mathbf{h}^1)$$

- Marginalization yields *P*(x), intractable in practice except for very small models

Sigmoid Belief Networks

$$P(\mathbf{x}, \mathbf{h}^1, \ldots, \mathbf{h}^l) = P(\mathbf{h}^l)\left(\prod_{k=1}^{l-1} P(\mathbf{h}^k|\mathbf{h}^{k+1})\right)P(\mathbf{x}|\mathbf{h}^1)$$

- The top level prior is chosen as factorizable:

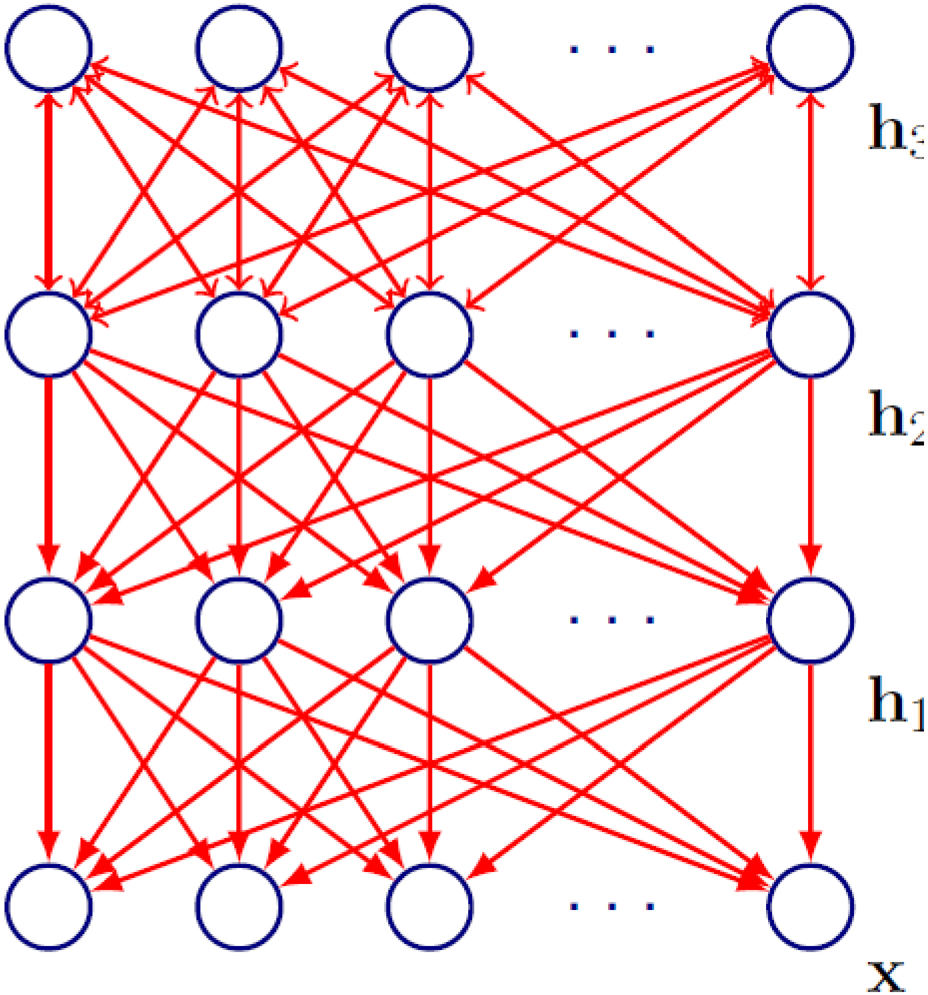
  $$P(\mathbf{h}^l) = \prod_i P(\mathbf{h}_i^l)$$

- A single (Bernoulli) parameter is needed for each h_i in case of binary units
- Deep Belief Networks are like Sigmoid Belief Networks except for the top two layers

Sigmoid Belief Networks

- General case models are called Helmholtz Machines
- Two key references:
  - G. E. Hinton, P. Dayan, B. J. Frey, R. M. Neal: The Wake-Sleep Algorithm for Unsupervised Neural Networks, In Science, 1995
  - R. M. Neal: Connectionist Learning of Belief Networks, In Artificial Intelligence, 1992

Deep Belief Networks



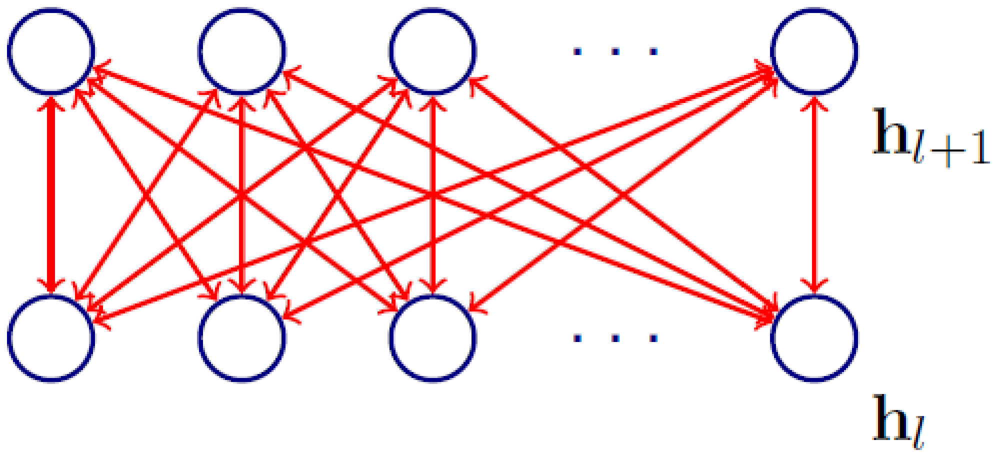
- The top two layers now have undirected edges

Deep Belief Networks

- The joint probability changes as:

$$P(\mathbf{x}, \mathbf{h}^1, \ldots, \mathbf{h}^l) = P(\mathbf{h}^l, \mathbf{h}^{l-1}) \Big(\prod_{k=1}^{l-2} P(\mathbf{h}^k | \mathbf{h}^{k+1}) \Big) P(\mathbf{x} | \mathbf{h}^1)$$

Deep Belief Networks



- The top two layers are a Restricted Boltzmann Machine (RBM)
- A RBM has the joint distribution:

$$P(\mathbf{h}^{l+1}, \mathbf{h}^{l}) \propto \exp(\mathbf{b}'\mathbf{h}^{l-1} + \mathbf{c}'\mathbf{h}^{l} + \mathbf{h}^{l} W \mathbf{h}^{l-1})$$

- We will return to RBMs and training procedures in a while, but the mathematical machinery will make our task easier

Greedy Layer-wise Training of DBNs

- Reference: G. E. Hinton, S. Osindero and Y-W Teh: A Fast Learning Algorithm for Deep Belief Networks, In Neural Computation, 2006.
- First Step: Construct a RBM with input **x** and a hidden layer **h**, train the RBM
- Stack another layer on top of the RBM to form a new RBM. Fix W^1, sample from $P(h^1|x)$, train W^2 as RBM
- Continue till *k* layers
- Implicitly defines *P*(x) and P(h) (variational bound justifies layerwise training)
- Can then be discriminatively fine-tuned using backpropagation

Energy Based Models

- Energy-Based Models assign a scalar energy with every configuration of variables under consideration
- Learning: Change the energy function so that its final shape has some desirable properties
- We can define a probability distribution through an energy:

$$P(\mathbf{x}) = \frac{\exp^{-(\text{Energy}(\mathbf{x}))}}{Z}$$

- Energies are in the log-probability domain:

$$\text{Energy}(\mathbf{x}) = \log \frac{1}{(ZP(\mathbf{x}))}$$

Energy Based Models

$$P(\mathbf{x}) = \frac{\exp^{-(\text{Energy}(\mathbf{x}))}}{Z}$$

- Z is a normalizing factor called the Partition Function

$$Z = \sum_{\mathbf{x}} \exp(-\text{Energy}(\mathbf{x}))$$

- How do we specify the energy function?

Product of Experts Formulation

- In this formulation, the energy function is:

$$\text{Energy}(\mathbf{x}) = \sum_i f_i(\mathbf{x})$$

- Therefore:

$$P(\mathbf{x}) = \frac{\exp^{-(\sum_i f_i(\mathbf{x}))}}{Z}$$

- We have the product of experts:

$$P(\mathbf{x}) \propto \prod_i P_i(\mathbf{x}) \propto \prod_i \exp^{(-f_i(\mathbf{x}))}$$

Product of Experts Formulation

$$P(\mathbf{x}) \propto \prod_i P_i(\mathbf{x}) \propto \prod_i \exp^{(-f_i(\mathbf{x}))}$$

- Every expert f_i can be seen as enforcing a constraint on x
- If f_i is large => P_i(x) is small i.e. the expert thinks x is implausible (constraint violated)
- If f_i is small => P_i(x) is large i.e. the expert thinks x is plausible (constraint satisfied)
- Contrast this with mixture models

Latent Variables

- x is observed, let's say **h** are hidden factors that explain x
- The probability then becomes:

$$P(\mathbf{x}, \mathbf{h}) = \frac{\exp^{-(\text{Energy}(\mathbf{x},\mathbf{h}))}}{Z}$$

- We only care about the marginal:

$$P(\mathbf{x}) = \sum_{\mathbf{h}} \frac{\exp^{-(\text{Energy}(\mathbf{x},\mathbf{h}))}}{Z}$$

Latent Variables

$$P(\mathbf{x}) = \sum_{\mathbf{h}} \frac{\exp^{-(\text{Energy}(\mathbf{x},\mathbf{h}))}}{Z}$$

- We introduce another term in analogy from statistical physics: free energy:

$$P(\mathbf{x}) = \frac{\exp^{-(\text{FreeEnergy}(\mathbf{x}))}}{Z}$$

- Free Energy is just a marginalization of energies in the log-domain:

$$\text{FreeEnergy}(\mathbf{x}) = -\log \sum_{\mathbf{h}} \exp^{-(\text{Energy}(\mathbf{x},\mathbf{h}))}$$

Latent Variables

$$P(\mathbf{x}) = \frac{\exp^{-(\mathsf{FreeEnergy}(\mathbf{x}))}}{Z}$$

- Likewise, the partition function:

$$Z = \sum_{\mathbf{x}} \exp^{-\mathsf{FreeEnergy}(\mathbf{x})}$$

- We have an expression for *P*(x) (and hence for the data log-likelihood). Let us see how the gradient looks like

Data Log-Likelihood Gradient

$$P(\mathbf{x}) = \frac{\exp^{-(\mathsf{FreeEnergy}(\mathbf{x}))}}{Z}$$

- The gradient is simply working from the above:

$$\frac{\partial \log P(\mathbf{x})}{\partial \theta} = -\frac{\partial \mathsf{FreeEnergy}(\mathbf{x})}{\partial \theta} + \frac{1}{Z} \sum_{\tilde{\mathbf{x}}} \exp^{-(\mathsf{FreeEnergy}(\tilde{\mathbf{x}}))} \frac{\partial \mathsf{FreeEnergy}(\tilde{\mathbf{x}})}{\partial \theta}$$

- Note that $P(\tilde{\mathbf{x}}) = \exp^{-(\mathsf{FreeEnergy}(\tilde{\mathbf{x}}))}$

Data Log-Likelihood Gradient

- The expected log-likelihood gradient over the training set has the following form:

$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = \mathbb{E}_{\tilde{P}}\left[\frac{\partial \mathsf{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \mathsf{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

Data Log-Likelihood Gradient

$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = \mathbb{E}_{\tilde{P}}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

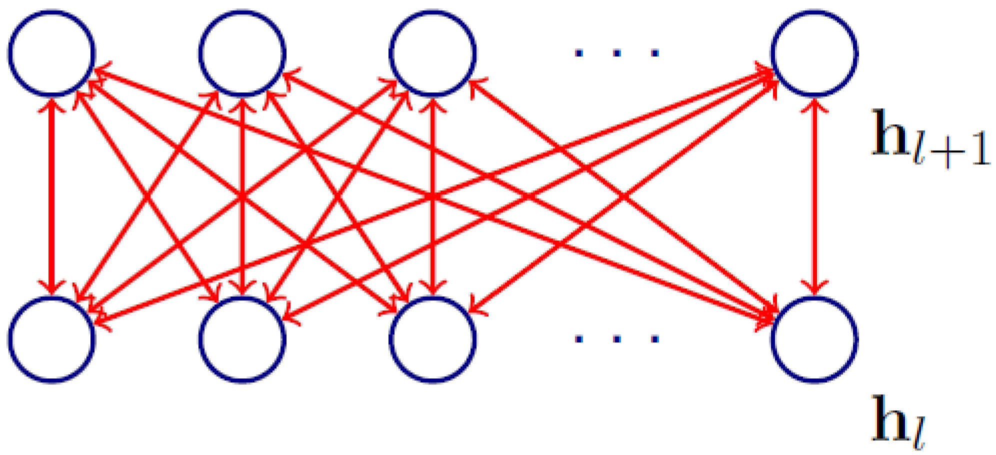
- $\tilde{P}$ is the empirical training distribution
- Easy to compute!

Data Log-Likelihood Gradient

$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = \mathbb{E}_{\tilde{P}}\left[\frac{\partial \mathsf{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \mathsf{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

- P is the model distribution (exponentially many configurations!)
- Usually very hard to compute!
- Resort to Markov Chain Monte Carlo to get a stochastic estimator of the gradient

Restricted Boltzmann Machines

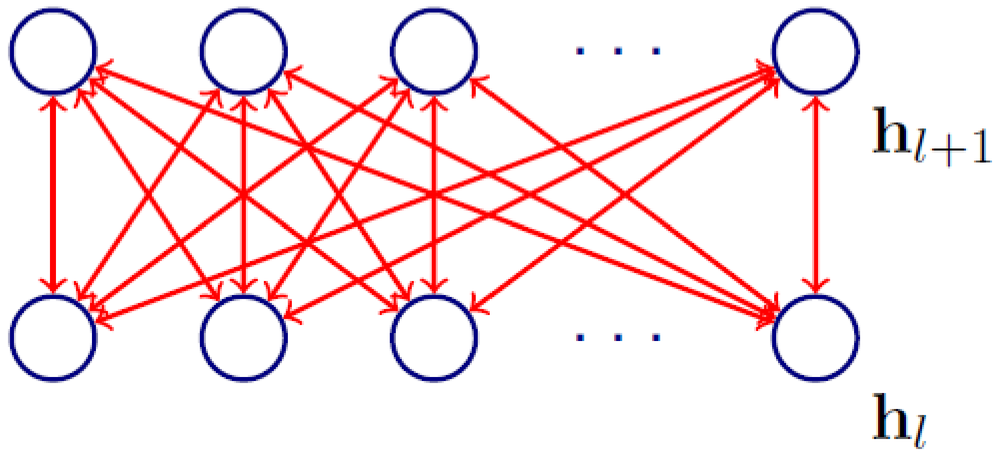


- Recall the form of energy:

$$\text{Energy}(\mathbf{x}, \mathbf{h}) = -\mathbf{b}^T\mathbf{x} - \mathbf{c}^T\mathbf{h} - \mathbf{h}^T W \mathbf{x}$$

- Originally proposed by Smolensky (1987) who called them Harmoniums as a special case of Boltzmann Machines

Restricted Boltzmann Machines



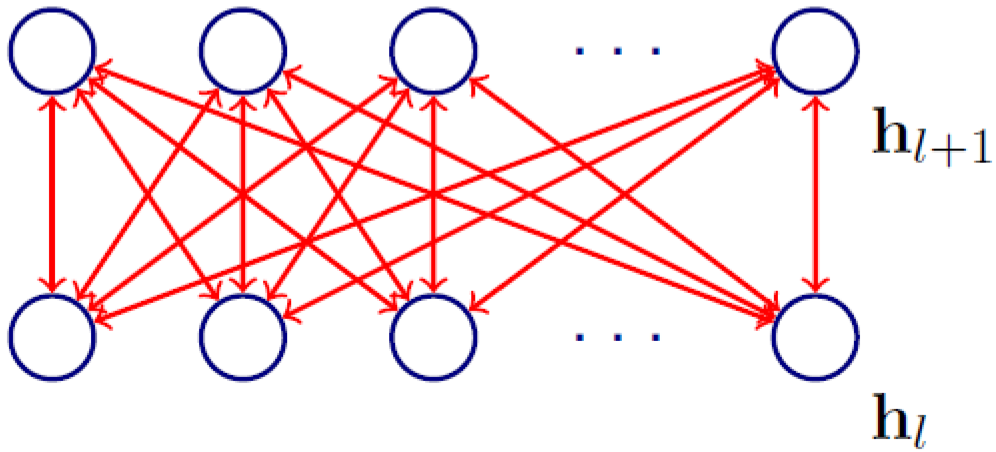
- As seen before, the Free Energy can be computed efficiently:

$$\text{FreeEnergy}(\mathbf{x}) = -\mathbf{b}^T\mathbf{x} - \sum_i \log \sum_{\mathbf{h}_i} \exp^{\mathbf{h}_i(\mathbf{c}_i + W_i \mathbf{x})}$$

- The conditional probability:

$$P(\mathbf{h}|\mathbf{x}) = \frac{\exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\mathbf{h} + \mathbf{h}^T W \mathbf{x}\right)}{\sum_{\tilde{\mathbf{h}}} \exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\tilde{\mathbf{h}} + \tilde{\mathbf{h}}^T W \mathbf{x}\right)} = \prod_i P(\mathbf{h}_i|\mathbf{x})$$

Restricted Boltzmann Machines



- x and h play symmetric roles:

$$P(\mathbf{x}|\mathbf{h}) = \prod_i P(\mathbf{x}_i|\mathbf{h})$$

- The common transfer (for the binary case):

$$P(\mathbf{h}_i = 1|\mathbf{x}) = \sigma(\mathbf{c_i} + W_i\mathbf{x})$$

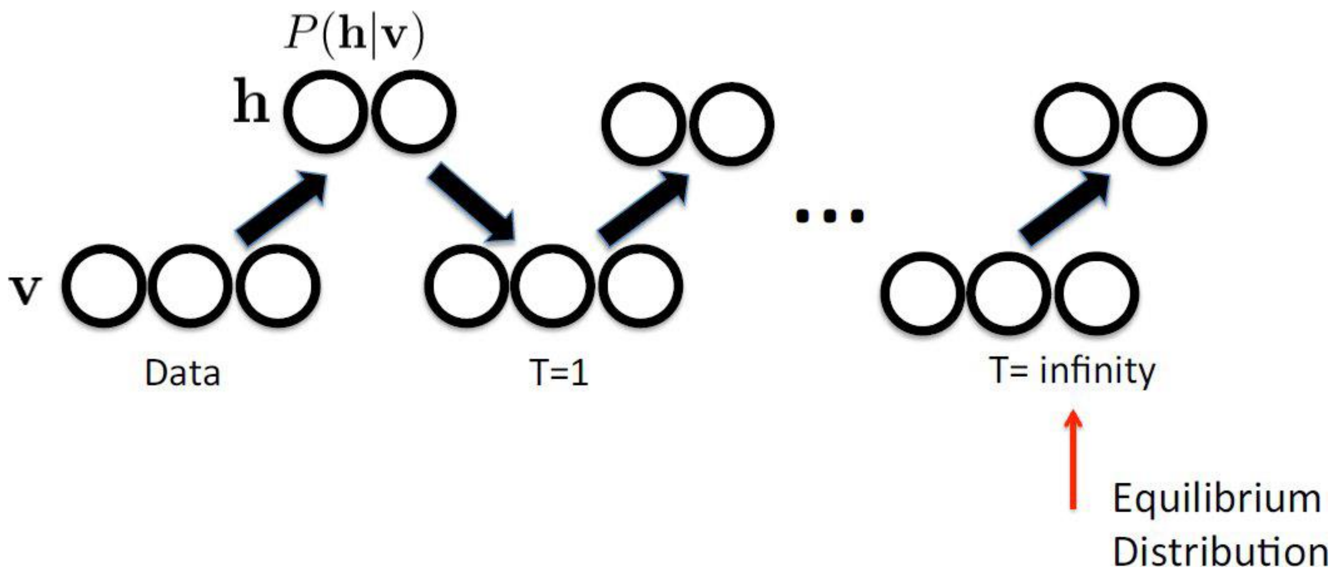
$$P(\mathbf{x}_j = 1|\mathbf{h}) = \sigma(\mathbf{b_j} + W_{:,j}^T\mathbf{h})$$

Approximate Learning and Gibbs Sampling

$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = \mathbb{E}_{\tilde{P}}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

- We saw the expression for Free Energy for a RBM. But the second term was intractable. How do learn in this case?
- Replace the average over all possible input configurations by samples
- Run Markov Chain Monte Carlo (Gibbs Sampling):
- First sample $x_1 \sim P(x)$, then $h_1 \sim P(h|x_1)$, then $X_2 \sim P(x|h_1)$, then $h_2 \sim P(h|x_2)$ till x_{k+1}

Approximate Learning, Alternating Gibbs Sampling



- We have already seen: $P(\mathbf{x}|\mathbf{h}) = \prod_i P(\mathbf{x}_i|\mathbf{h})$

  $$P(\mathbf{h}|\mathbf{x}) = \prod_i P(\mathbf{h}_i|\mathbf{x})$$

- With: $P(\mathbf{h}_i = 1|\mathbf{x}) = \sigma(\mathbf{c_i} + W_i\mathbf{x})$ and

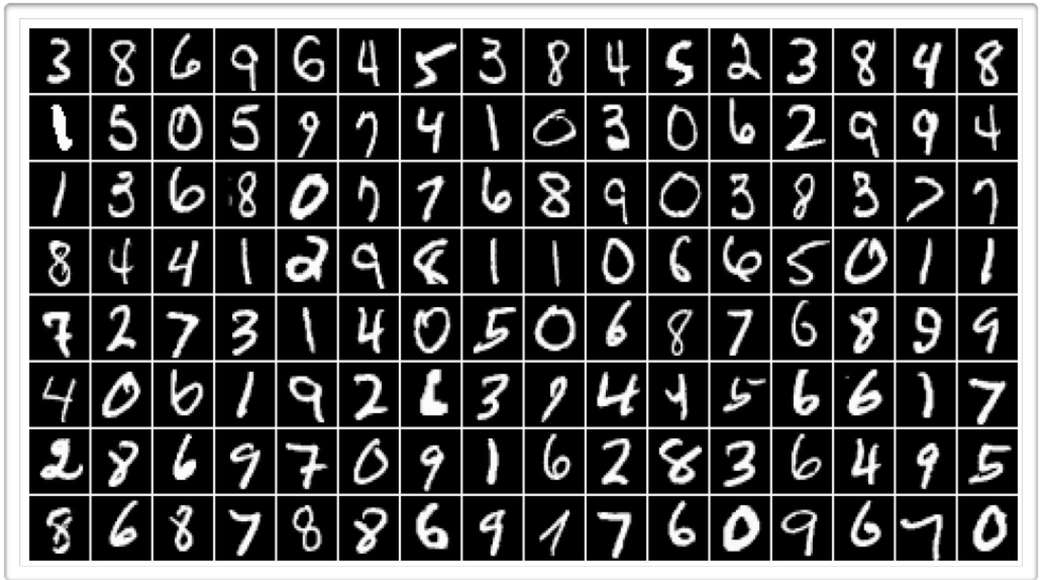
  $$P(\mathbf{x}_j = 1|\mathbf{h}) = \sigma(\mathbf{b_j} + W_{:,j}^T\mathbf{h})$$

Training RBM: Contrastive Divergence Algorithm

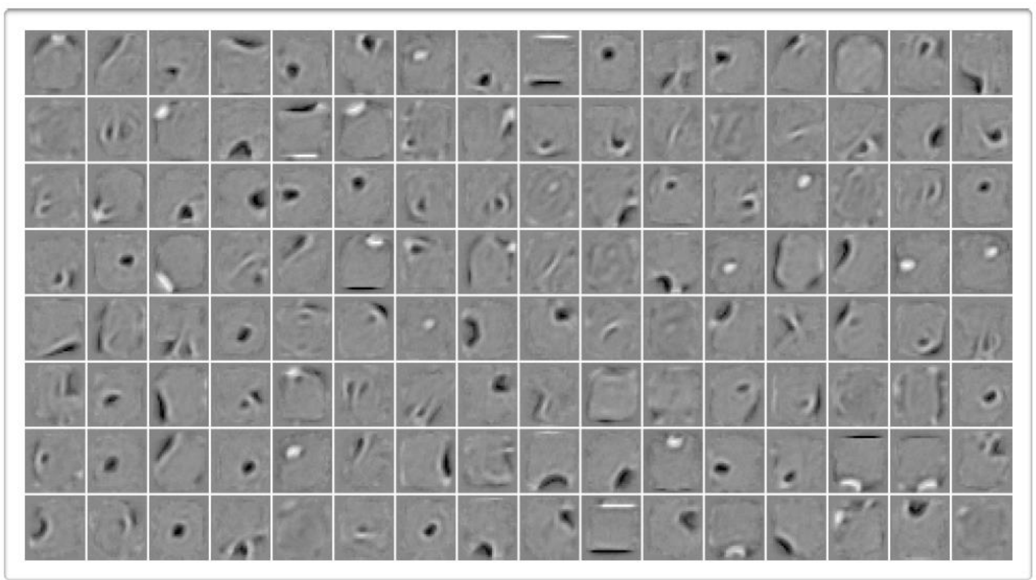
- Start with a training example on the visible units
- Update all the hidden units in parallel
- Update all the visible units in parallel to obtain a reconstruction
- Update all the hidden units again
- Update model parameters
- Aside: Easy to extend RBM (and contrastive divergence) to the continuous case

Example: MNIST

Original images:



Learned features:



(Larochelle et al., JMLR 2009)

Acknowledgement

Some of the materials in these slides are drawn inspiration from:

- Shubhendu Trivedi and Risi Kondor, University of Chicago, Deep Learning Course
- Hung-yi Lee, National Taiwan University, Machine Learning and having it Deep and Structured course
- Xiaogang Wang, The Chinese University of Hong Kong, Deep Learning Course
- Fei-Fei Li, Standord University, CS231n Convolutional Neural Networks for Visual Recognition course

Next time

- Generative Model (2)

Questions?

Thank You !