10417/10617 Intermediate Deep Learning: Fall2019

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https://deeplearning-cmu-10417.github.io/

Sparse Coding

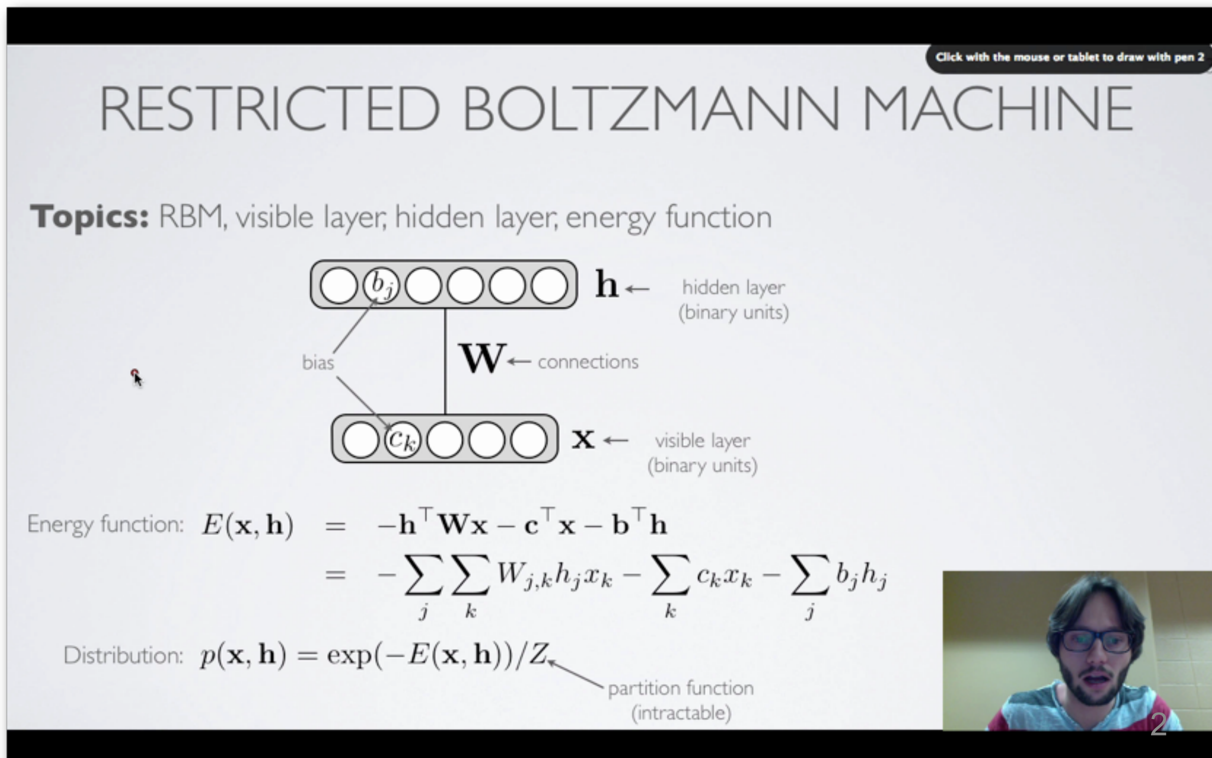
Neural Networks Online Course

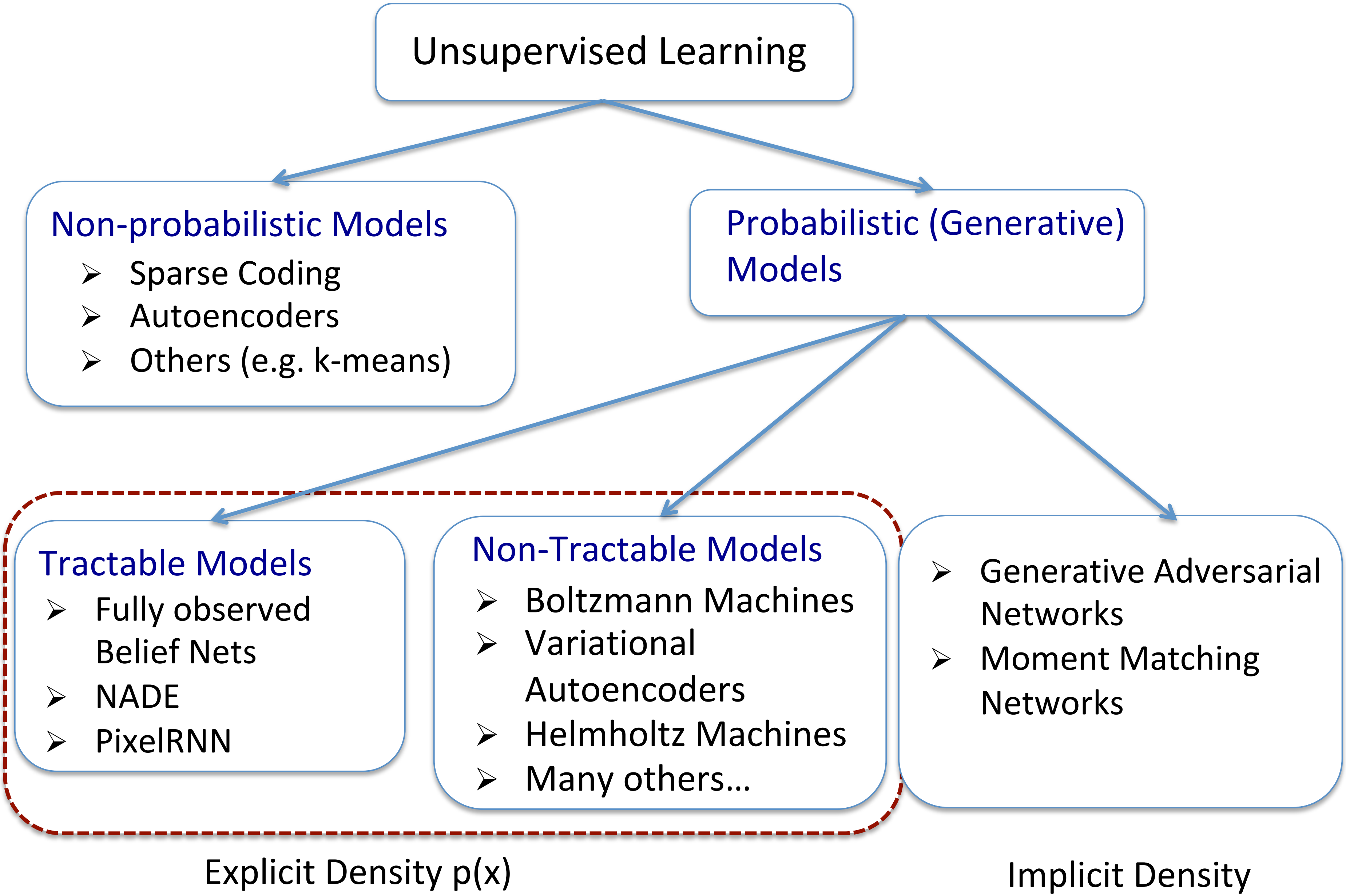
- **Disclaimer**: Much of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks:

http://info.usherbrooke.ca/hlarochelle/neural_networks

- Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.

- We will use his material for some of the other lectures.




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

Unsupervised Learning

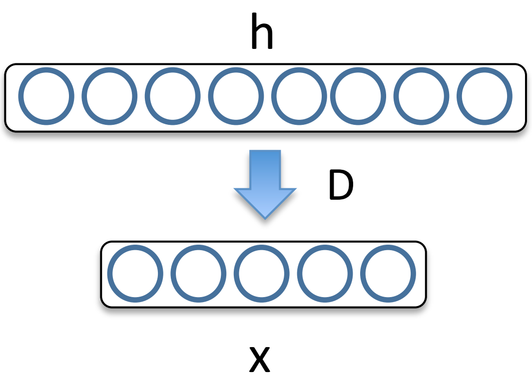
- Unsupervised learning: we only use the inputs $\mathbf{x}^{(t)}$ for learning
    - automatically extract meaningful features for your data
    - leverage the availability of unlabeled data
    - add a data-dependent regularizer to training ($-\log p(\mathbf{x}^{(t)})$)

- We consider 3 models for unsupervised learning that will form the basic building blocks for deeper models:
    - Restricted Boltzmann Machines
    - Autoencoders
    - Sparse coding models

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 good 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 good reconstruct the original input $\mathbf{x}^{(t)}$

- In other words:

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

Sparsity vs. reconstruction control

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

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

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:

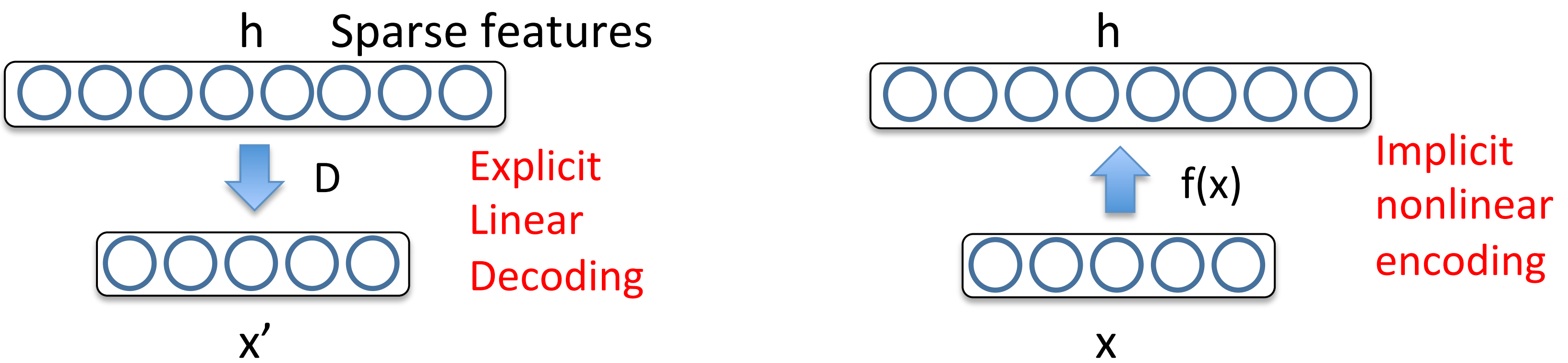
$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} ||\mathbf{x}^{(t)} - \mathbf{D}\ \mathbf{h}^{(t)}||_2^2 + \lambda ||\mathbf{h}^{(t)}||_1$$

  - D is equivalent to the autoencoder output weight matrix
  - However, $\mathbf{h}(\mathbf{x}^{(t)})$ is now a complicated function of $\mathbf{x}^{(t)}$
  - Encoder is the minimization problem:

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

Interpreting Sparse Coding

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

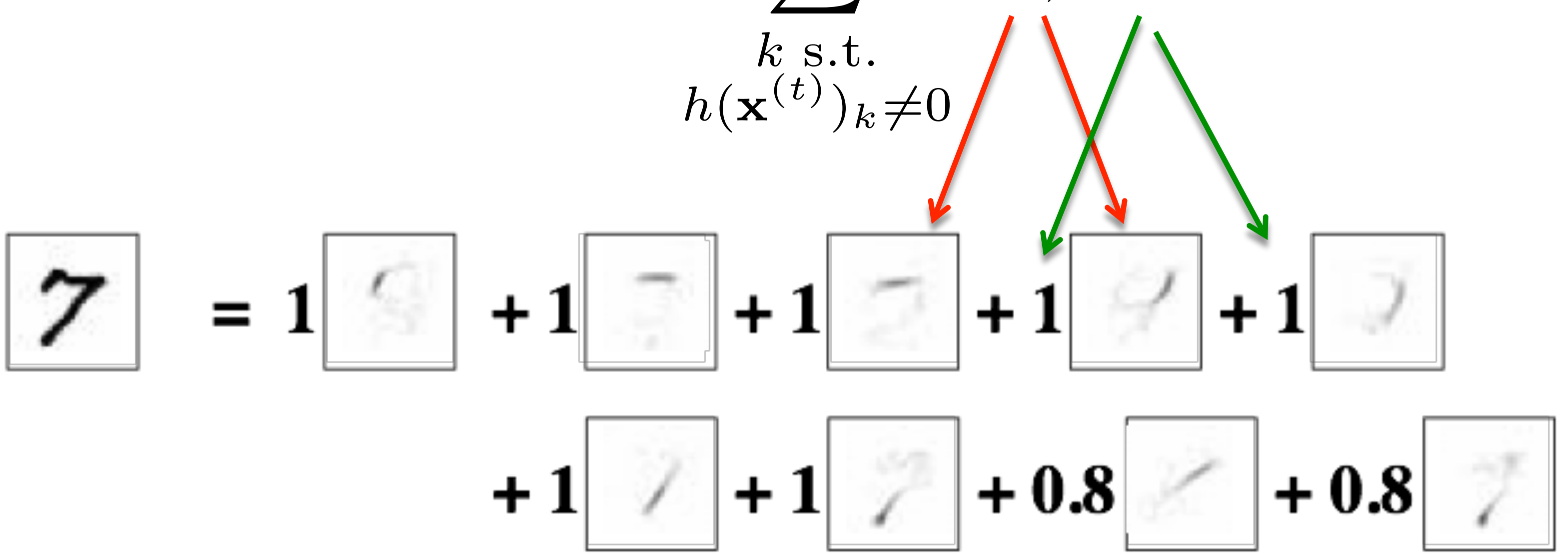


- Sparse, over-complete representation **h.**
- Encoding **h** = f(**x**) is implicit and nonlinear function of **x**.
- Reconstruction (or decoding) **x’** = Dh is linear and explicit.

Sparse Coding

- We can also write:

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

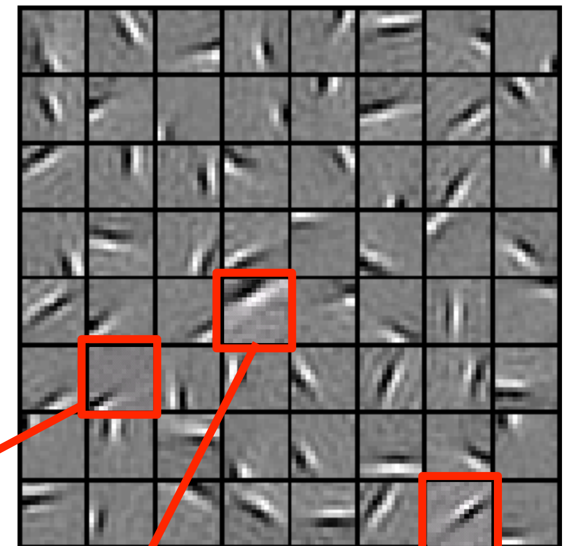


- ➢ D is often referred to as Dictionary
- ➢ In certain applications, we know what dictionary matrix to use
- ➢ In many cases, we have to learn it

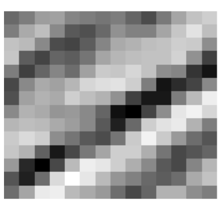
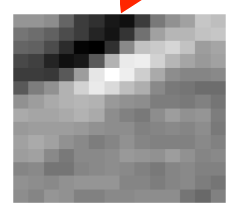
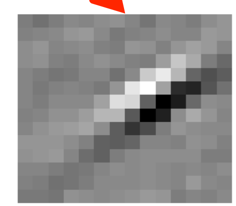
Sparse Coding

Natural Images

Learned bases: “Edges”



New example

 $= 0.8 *$  $+ 0.3 *$  $+ 0.5 *$ 

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

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

Slide Credit: Honglak Lee

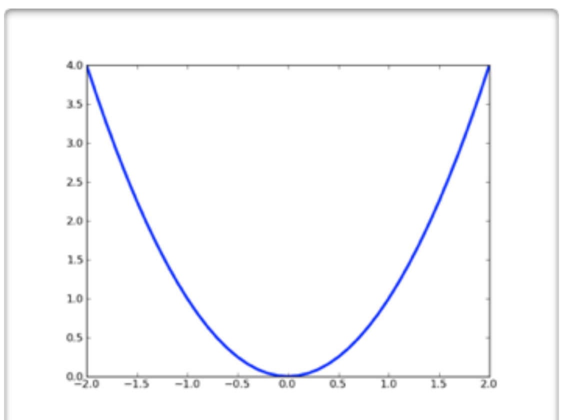
Inference

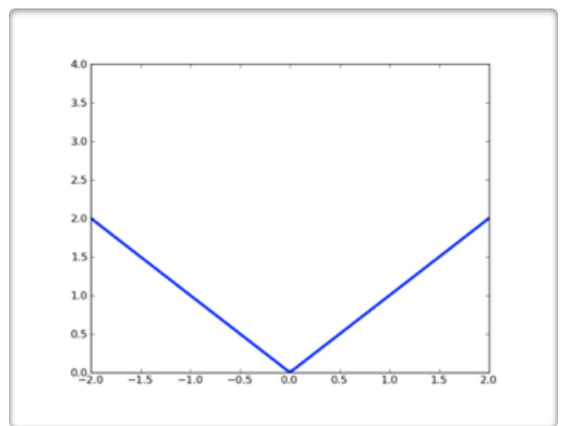
- Given dictionary D , how do we compute $\mathbf{h}(\mathbf{x}^{(t)})$?

  - We need to optimize:

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

  - This is Lasso.





  - We could use a gradient descent method:

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

Inference

- For a single hidden unit:

$$\frac{\partial}{\partial h_k^{(t)}} l(\mathbf{x}^{(t)}) = (\mathbf{D}_{\cdot,k})^\top (\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)}) + \lambda \operatorname{sign}(h_k^{(t)})$$

  - issue: L1 norm not differentiable at 0
  - very unlikely for gradient descent to "land" on $h_k^{(t)} = 0$ (even if it's the solution)

- Solution: if $h_k^{(t)}$ changes sign because of L1 norm gradient, clamp to 0.

Inference

- For a single hidden unit:

$$\frac{\partial}{\partial h_k^{(t)}} l(\mathbf{x}^{(t)}) = (\mathbf{D}_{\cdot,k})^\top (\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)}) + \lambda\,\mathrm{sign}(h_k^{(t)})$$

- Solution: if $h_k^{(t)}$ changes sign because of L1 norm gradient, clamp to 0.

- Each hidden unit update would be performed as follows:

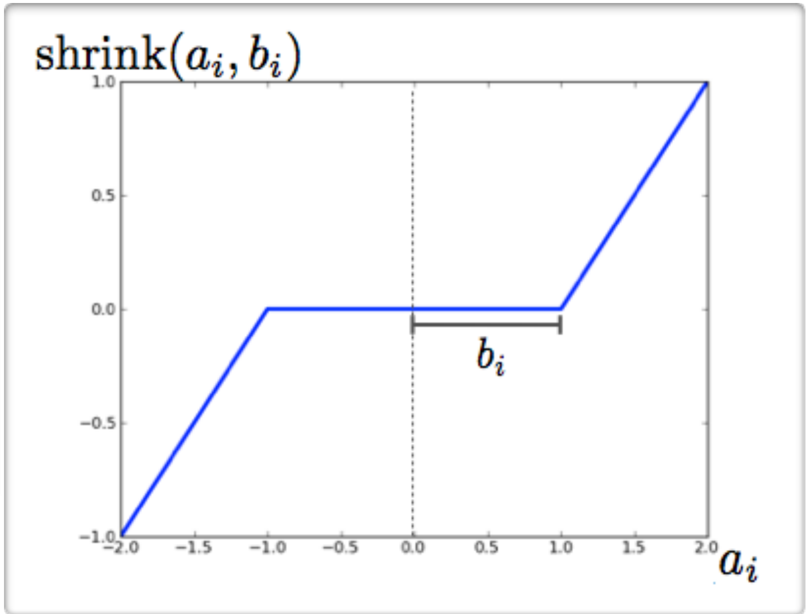
  - $h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha (\mathbf{D}_{\cdot,k})^\top (\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)})$ Update from reconstruction
  - If $\mathrm{sign}(h_k^{(t)}) \neq \mathrm{sign}(h_k^{(t)} - \alpha\,\lambda\,\mathrm{sign}(h_k^{(t)}))$ then $h_k^{(t)} \Longleftarrow 0$
  - Else $h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha\,\lambda\,\mathrm{sign}(h_k^{(t)})$

Update sparsity term

ISTA Algorithm

- This process corresponds to the ISTA (Iterative Shrinkage and Thresholding) Algorithm:

> - Initialize $\mathbf{h}^{(t)}$ (for example to 0)
> - While $\mathbf{h}^{(t)}$ has not converged
>
> $$\mathbf{h}^{(t)} \Longleftarrow \mathbf{h}^{(t)} - \alpha\, \mathbf{D}^\top (\mathbf{D}\, \mathbf{h}^{(t)} - \mathbf{x}^{(t)})$$
>
> $$\mathbf{h}^{(t)} \Longleftarrow \mathrm{shrink}(\mathbf{h}^{(t)}, \alpha\, \lambda)$$



where

$$\mathrm{shrink}(\mathbf{a}, \mathbf{b}) = [\ldots, \mathrm{sign}(a_i)\ \max(|a_i| - b_i, 0), \ldots]$$

- Will converge if $\frac{1}{\alpha}$ is bigger than the largest eigenvalue of $\mathbf{D}^\top \mathbf{D}$

ISTA Algorithm

- ISTA updates all hidden units simultaneously
  - this is wasteful if many hidden units have already converged

- Idea: update only the “most promising” hidden unit
  - see coordinate descent algorithm in Learning Fast Approximations of Sparse Coding (Gregor and Lecun, 2010).
  - this algorithm has the advantage of not requiring a learning rate α

Dictionary Learning I

- Remember our optimization problem:

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

- Let us first assume that $\mathbf{h}(\mathbf{x}^{(t)})$ does not depend on D
  - ➢ We then minimize:

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

  - ➢ we must also constrain the columns of D to be of unit norm

Dictionary Learning I

- We can use projected gradient descent algorithm.

- While D has not converged:
  - Perform gradient update of D

$$\mathbf{D} \Longleftarrow \mathbf{D} + \alpha \frac{1}{T} \sum_{t=1}^{T} (\mathbf{x}^{(t)} - \mathbf{D}\, \mathbf{h}(\mathbf{x}^{(t)}))\, \mathbf{h}(\mathbf{x}^{(t)})^{\top}$$

  - Renormalize the columns of D
  - For each column of D:

$$\mathbf{D}_{\cdot,j} \Longleftarrow \frac{\mathbf{D}_{\cdot,j}}{||\mathbf{D}_{\cdot,j}||_2}$$

Dictionary Learning II

- An alternative method is to solve for each column $\mathbf{D}_{\cdot,j}$ in cycle.

➢ setting the gradient for $\mathbf{D}_{\cdot,j}$ to zero, we have

$$
\begin{aligned}
0 &= \frac{1}{T}\sum_{t=1}^{T}(\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}(\mathbf{x}^{(t)}))\,h(\mathbf{x}^{(t)})_j \\
0 &= \sum_{t=1}^{T}\left(\mathbf{x}^{(t)} - \left(\sum_{i\neq j}\mathbf{D}_{\cdot,i}\,h(\mathbf{x}^{(t)})_i\right) - \mathbf{D}_{\cdot,j}\,h(\mathbf{x}^{(t)})_j\right)\,h(\mathbf{x}^{(t)})_j \\
\sum_{t=1}^{T}\mathbf{D}_{\cdot,j}h(\mathbf{x}^{(t)})_j^2 &= \sum_{t=1}^{T}\left(\mathbf{x}^{(t)} - \left(\sum_{i\neq j}\mathbf{D}_{\cdot,i}\,h(\mathbf{x}^{(t)})_i\right)\right)\,h(\mathbf{x}^{(t)})_j \\
\mathbf{D}_{\cdot,j} &= \frac{1}{\sum_{t=1}^{T}h(\mathbf{x}^{(t)})_j^2}\sum_{t=1}^{T}\left(\mathbf{x}^{(t)} - \left(\sum_{i\neq j}\mathbf{D}_{\cdot,i}\,h(\mathbf{x}^{(t)})_i\right)\right)\,h(\mathbf{x}^{(t)})_j
\end{aligned}
$$

➢ Note that we don’t need to specify a learning rate to update D.

Dictionary Learning II

- An alternative method is to solve for each column $\mathbf{D}_{\cdot,j}$ in cycle.

  - We can rewrite

$$\mathbf{D}_{\cdot,j} = \frac{1}{\sum_{t=1}^{T} h(\mathbf{x}^{(t)})_j^2} \sum_{t=1}^{T} \left(\mathbf{x}^{(t)} - \left(\sum_{i \neq j} \mathbf{D}_{\cdot,i}\, h(\mathbf{x}^{(t)})_i \right) \right) h(\mathbf{x}^{(t)})_j$$

$$= \frac{1}{\sum_{t=1}^{T} h(\mathbf{x}^{(t)})_j^2} \left(\left(\sum_{t=1}^{T} \mathbf{x}^{(t)} h(\mathbf{x}^{(t)})_j \right) - \sum_{i \neq j} \mathbf{D}_{\cdot,i} \left(\sum_{t=1}^{T} h(\mathbf{x}^{(t)})_i h(\mathbf{x}^{(t)})_j \right) \right)$$

$$= \frac{1}{A_{j,j}} (\mathbf{B}_{\cdot,j} - \mathbf{D}\ \mathbf{A}_{\cdot,j} + \mathbf{D}_{\cdot,j} A_{j,j})$$

  - this way, we only need to store:

$$\mathbf{A} \Longleftarrow \textstyle\sum_{t=1}^{T} \mathbf{h}(\mathbf{x}^{(t)})\ \mathbf{h}(\mathbf{x}^{(t)})^\top$$

$$\mathbf{B} \Longleftarrow \textstyle\sum_{t=1}^{T} \mathbf{x}^{(t)}\ \mathbf{h}(\mathbf{x}^{(t)})^\top$$

Dictionary Learning II

- This leads to the following algorithm

> - While D has not converged:
>   - for each column $\mathbf{D}_{\cdot,j}$ perform updates
>
> $$\mathbf{D}_{\cdot,j} \Longleftarrow \frac{1}{A_{j,j}} \left(\mathbf{B}_{\cdot,j} - \mathbf{D}\ \mathbf{A}_{\cdot,j} + \mathbf{D}_{\cdot,j}\ A_{j,j}\right)$$
>
> $$\mathbf{D}_{\cdot,j} \Longleftarrow \frac{\mathbf{D}_{\cdot,j}}{||\mathbf{D}_{\cdot,j}||_2}$$

- This is referred to as a block-coordinate descent algorithm
  - a different block of variables are updated at each step
  - the "blocks" are the columns $\mathbf{D}_{\cdot,j}$

Learning Sparse Coding Model

- Putting it all together, we have the following algorithm, where learning alternates between inference and dictionary learning.

- While D has not converged:
    - find the sparse codes $\mathbf{h}(\mathbf{x}^{(t)})$ for all $\mathbf{x}^{(t)}$ in the training set with ISTA
    - Update the dictionary:

      $$\mathbf{A} \Longleftarrow \sum_{t=1}^{T} \mathbf{x}^{(t)} \, \mathbf{h}(\mathbf{x}^{(t)})^{\top}$$

      $$\mathbf{B} \Longleftarrow \sum_{t=1}^{T} \mathbf{h}(\mathbf{x}^{(t)}) \, \mathbf{h}(\mathbf{x}^{(t)})^{\top}$$
    - run block-coordinate descent algorithm to update D

- Similar in spirit to EM algorithm

ZCA Preprocessing

- Before running a sparse coding algorithm, it is beneficial to remove "obvious" structure from the data
  - ➢ normalize such that mean is 0 and covariance is the identity (whitening)
  - ➢ this will remove 1st and 2nd order statistical structure

- ZCA preprocessing
  - ➢ let the empirical mean be $\widehat{\boldsymbol{\mu}}$ and the empirical covariance matrix be $\widehat{\Sigma} = \mathbf{U}\Lambda\mathbf{U}^\top$ (in its eigenvalue/eigenvector representation)
  - ➢ ZCA transforms each input as follows:

$$\mathbf{x} \Longleftarrow \mathbf{U}\,\Lambda^{-\frac{1}{2}}\,\mathbf{U}^\top(\mathbf{x} - \widehat{\boldsymbol{\mu}})$$

ZCA Preprocessing

- After this transformation
  - the empirical mean is 0

$$
\begin{aligned}
& \frac{1}{T}\sum_t \mathbf{U}\,\Lambda^{-\frac{1}{2}}\,\mathbf{U}^\top(\mathbf{x}^{(t)} - \widehat{\boldsymbol{\mu}}) \\
= \quad & \mathbf{U}\,\Lambda^{-\frac{1}{2}}\,\mathbf{U}^\top\left(\left(\frac{1}{T}\sum_t \mathbf{x}^{(t)}\right) - \widehat{\boldsymbol{\mu}}\right) \\
= \quad & \mathbf{U}\,\Lambda^{-\frac{1}{2}}\,\mathbf{U}^\top\,(\widehat{\boldsymbol{\mu}} - \widehat{\boldsymbol{\mu}}) \\
= \quad & 0
\end{aligned}
$$

ZCA Preprocessing

- After this transformation
  - ➢ the empirical covariance matrix is the identity

$$
\begin{aligned}
& \frac{1}{T-1} \sum_t \left(\mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top (\mathbf{x}^{(t)} - \widehat{\boldsymbol{\mu}}) \right) \left(\mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top (\mathbf{x}^{(t)} - \widehat{\boldsymbol{\mu}}) \right)^\top \\
= \quad & \mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top \left(\frac{1}{T-1} \sum_t (\mathbf{x}^{(t)} - \widehat{\boldsymbol{\mu}})(\mathbf{x}^{(t)} - \widehat{\boldsymbol{\mu}}) \right)^\top \mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top \\
= \quad & \mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top\, \widehat{\Sigma}\, \mathbf{U} \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top \\
= \quad & \mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top\, \mathbf{U}\, \Lambda\, \mathbf{U}^\top\, \mathbf{U}\, \Lambda^{-\frac{1}{2}}\, \mathbf{U}^\top \\
= \quad & \mathrm{I}
\end{aligned}
$$

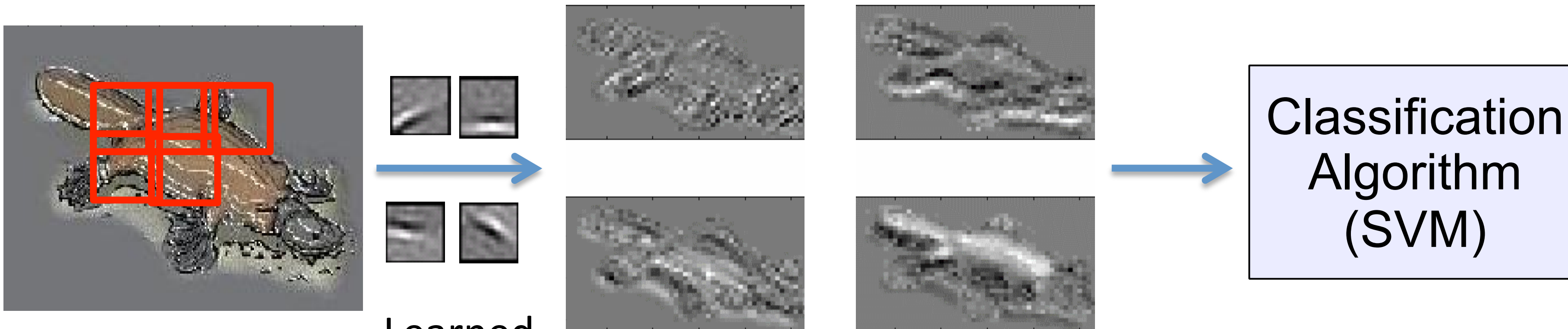
Feature Learning

- A sparse coding model can be used to extract features
  - given a labeled training set $\{(\mathbf{x}^{(t)}, y^{(t)})\}$
  - train sparse coding dictionary only on training inputs $\{\mathbf{x}^{(t)}\}$
  - this yields a dictionary $\mathbf{h}(\mathbf{x}^{(t)})$ from which to infer sparse codes
  - train your favorite classifier on transformed training set $\{(\mathbf{h}(\mathbf{x}^{(t)}), y^{(t)})\}$

- When classifying test input x
  - infer its sparse representation: $\mathbf{h}(\mathbf{x})$
  - feed it to the classifier

Image Classification

Evaluated on Caltech101 object category dataset.

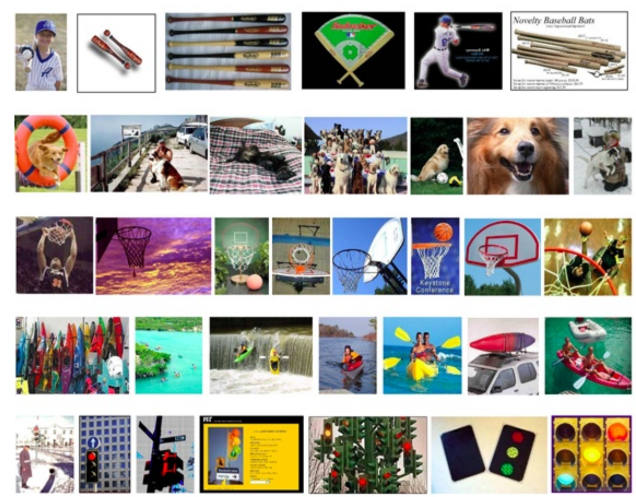


Input Image

Learned bases

Features (coefficients)

9K images, 101 classes

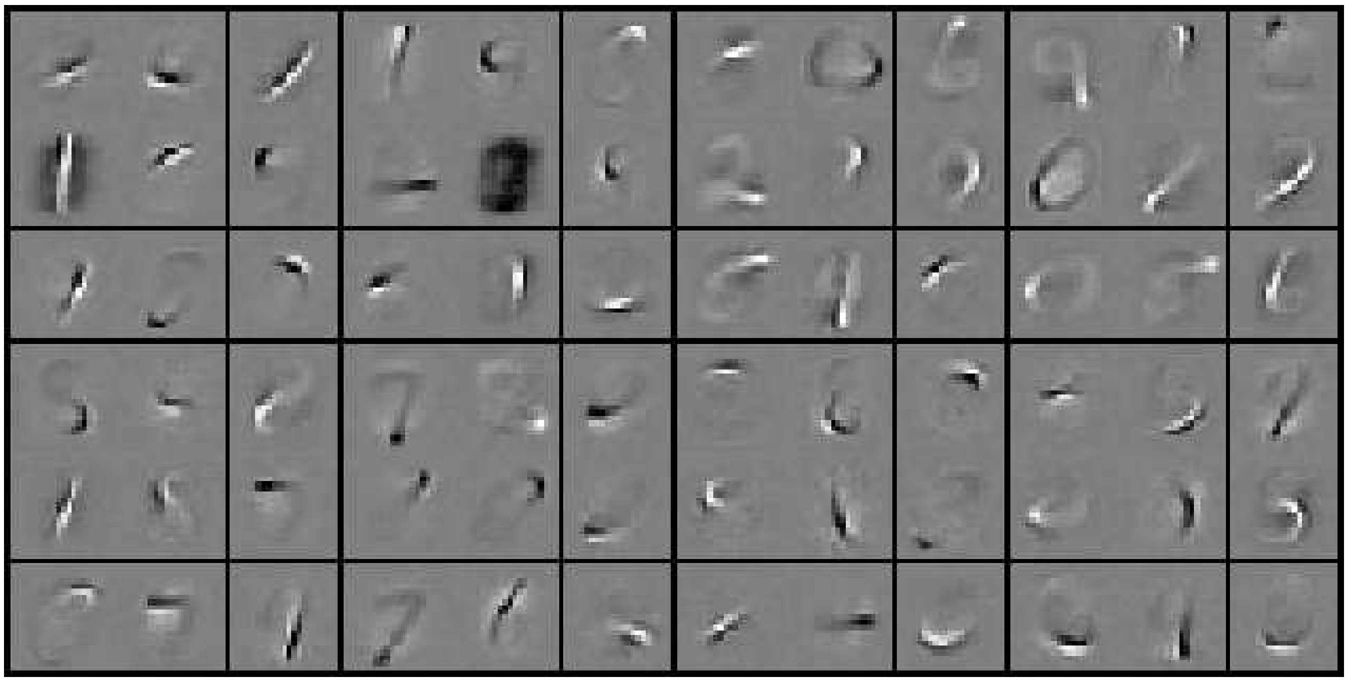


Algorithm	Accuracy
Baseline (Fei-Fei et al., 2004)	16%
PCA	37%
Sparse Coding	**47%**

Lee et al., NIPS 2006

Feature Learning

- Learned features on MNIST handwritten digits:



Self-taught Learning: Transfer Learning from Unlabeled DataRaina, Battle, Lee, Packer and Ng.

Self-Taught Learning

- Self-taught learning: when features trained on different input distribution

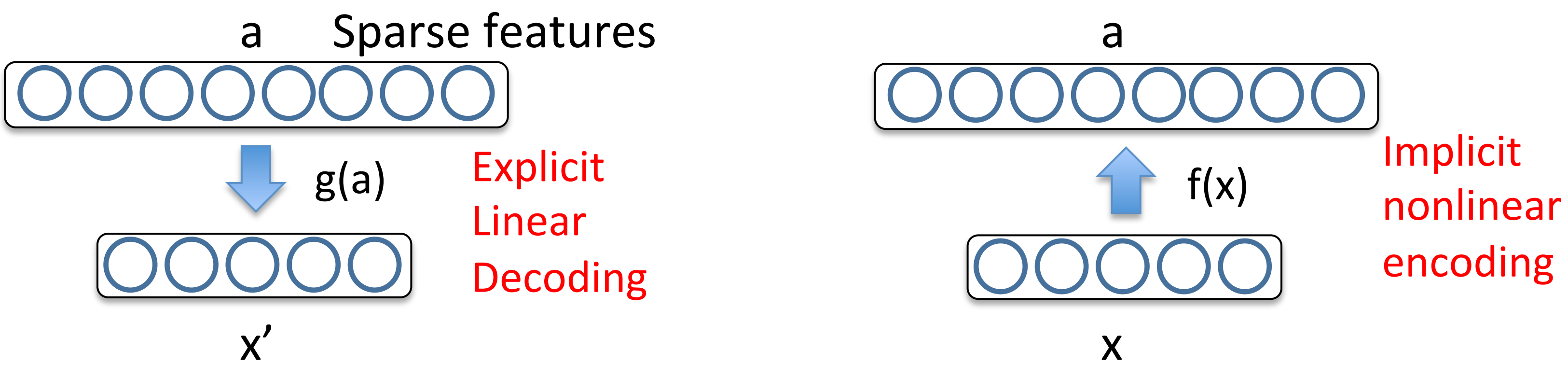
- Example:
  - train sparse coding dictionary on handwritten digits
  - use codes (features) to classify handwritten characters

Digits → English handwritten characters			
Training set size	Raw	PCA	Sparse coding
100	**39.8%**	25.3%	39.7%
500	54.8%	54.8%	**58.5%**
1000	61.9%	64.5%	**65.3%**

Self-taught Learning: Transfer Learning from Unlabeled DataRaina, Battle, Lee, Packer and Ng.

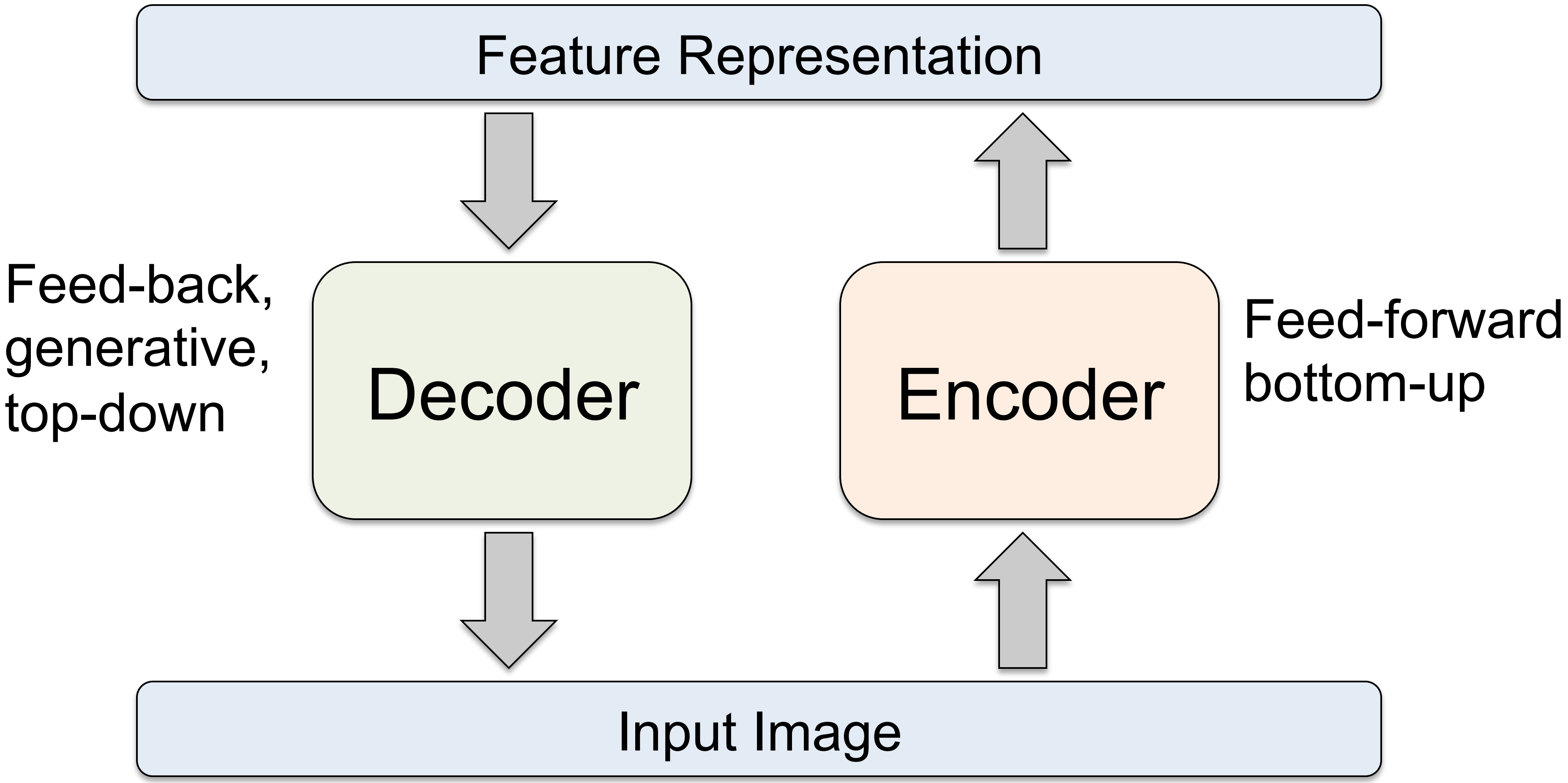
Interpreting Sparse Coding

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



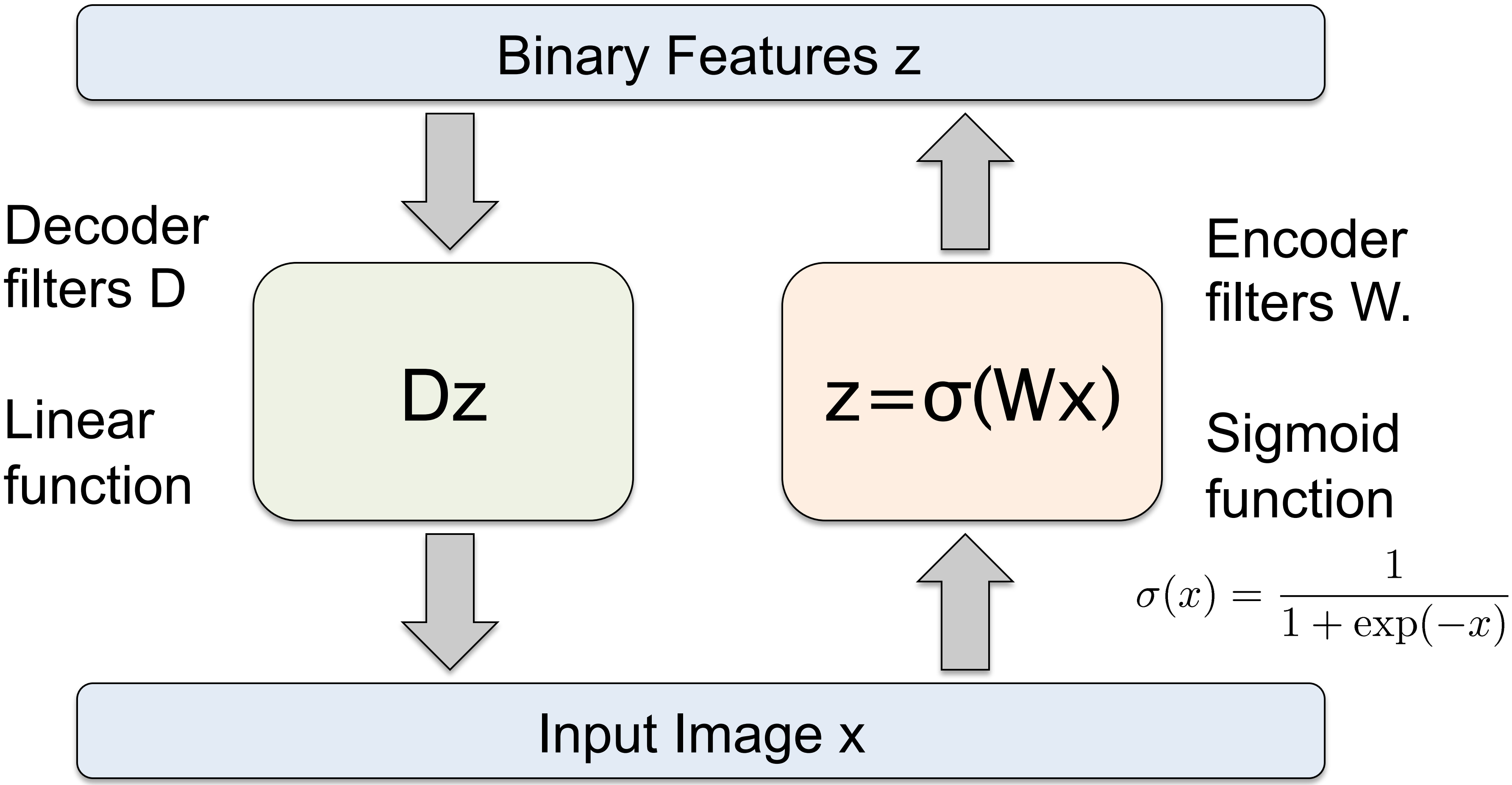
- Sparse, over-complete representation **a.**
- Encoding **a** = f(**x**) is implicit and nonlinear function of **x**.
- Reconstruction (or decoding) **x'** = g(**a**) is linear and explicit.

Autoencoder

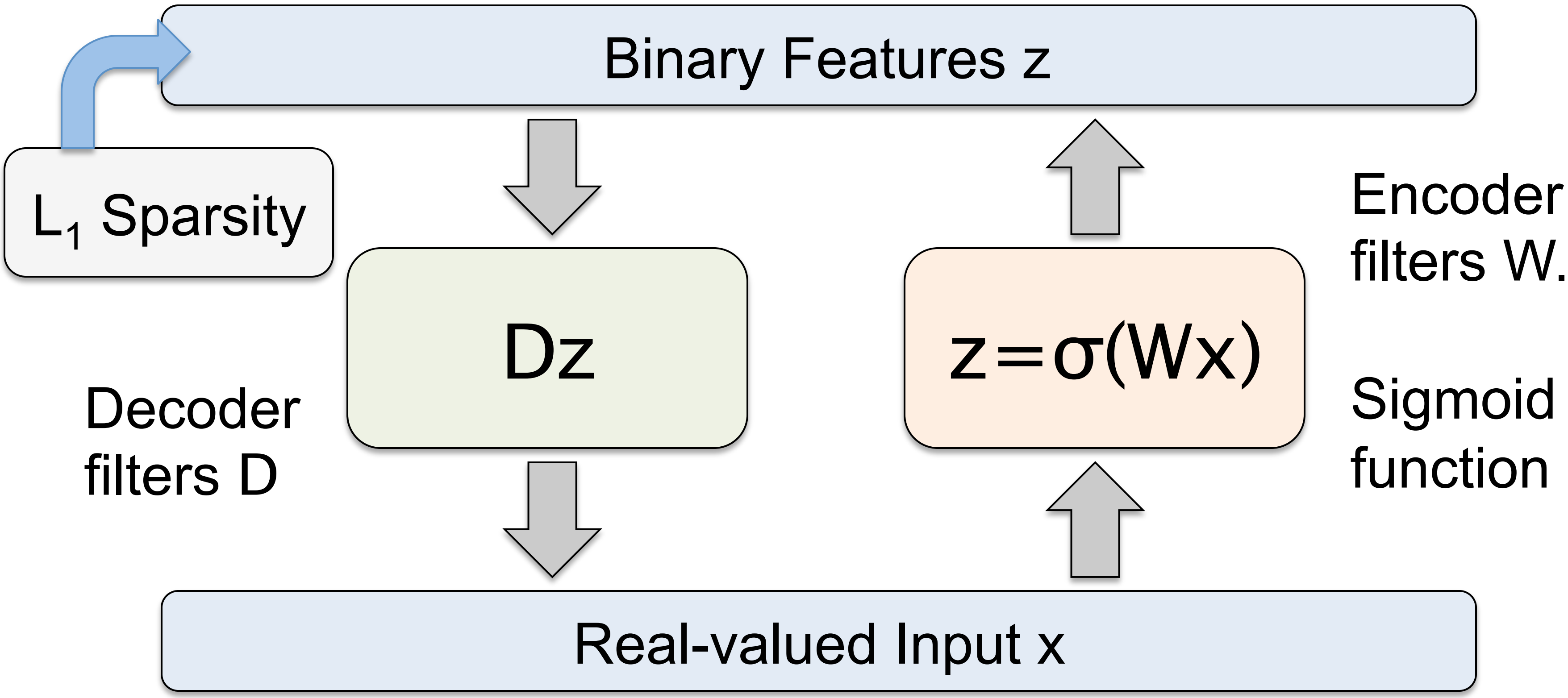


- Details of what goes insider the encoder and decoder matter!
- Need constraints to avoid learning an identity.

Autoencoder



Predictive Sparse Decomposition

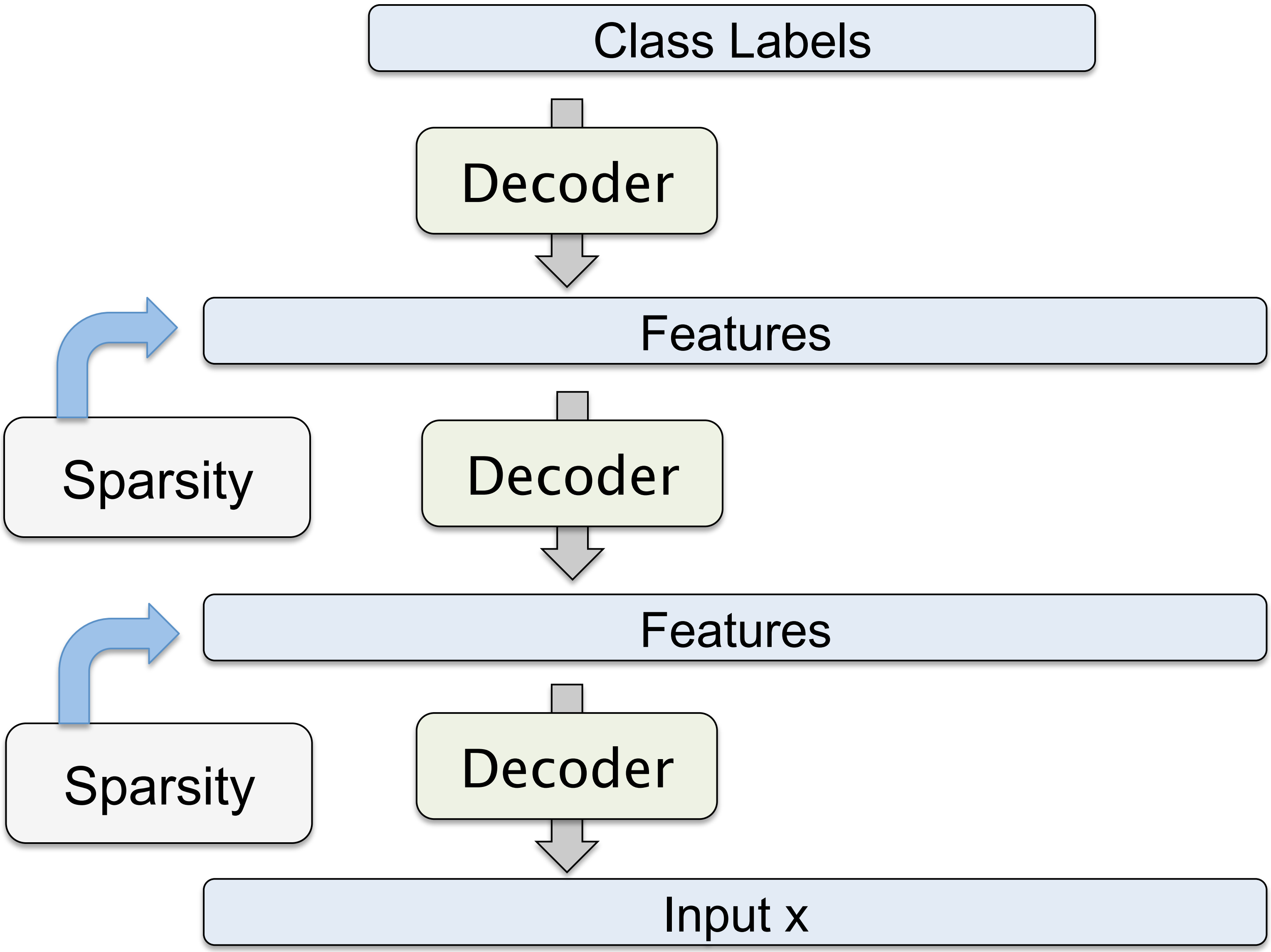


At training time

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

Kavukcuoglu et al., ‘09

Stacked Sparse Coding?



Modeling Image Patches

- Natural image patches:
  - small image regions extracted from an image of nature (forest, grass, ...)

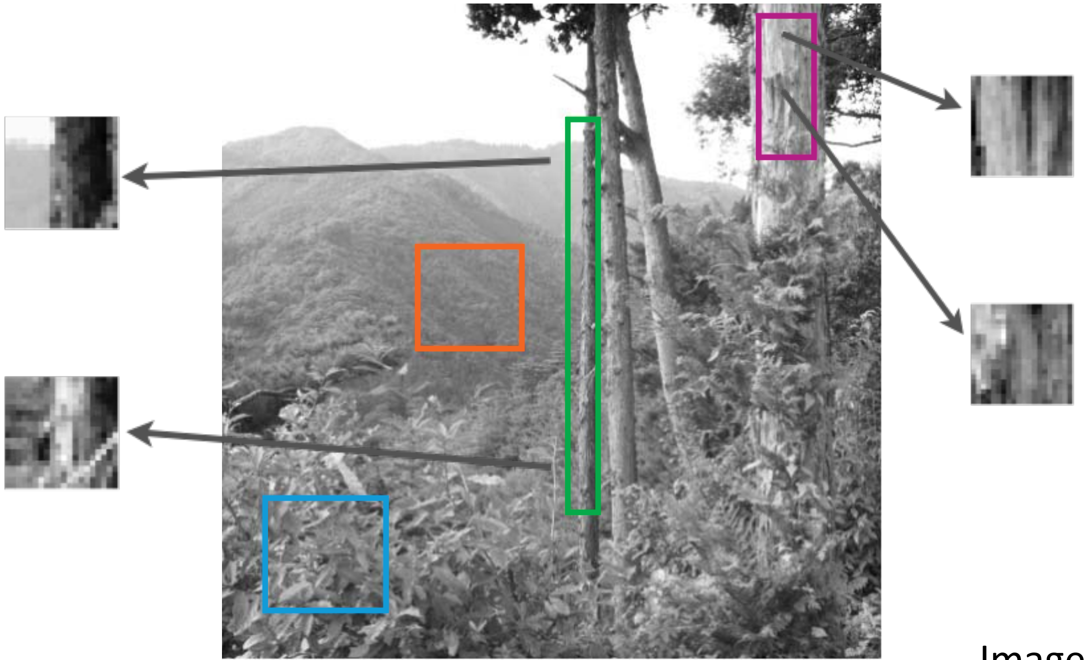
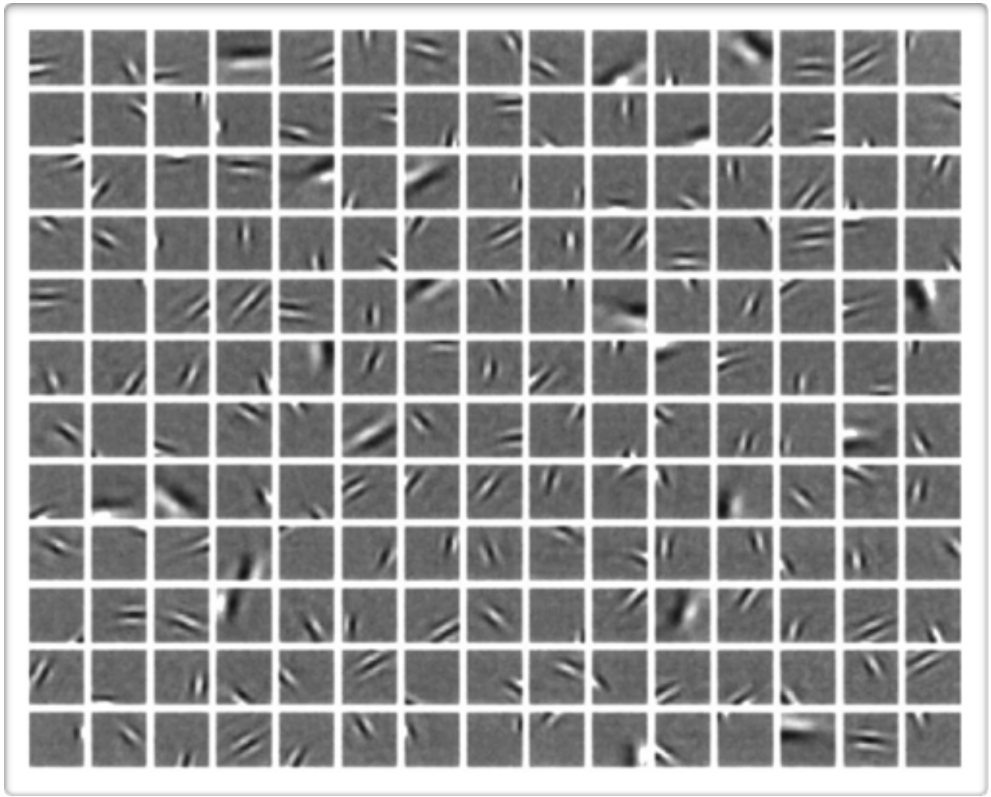


Image taken from:
Emergence of complex cell properties
by learning to generalize in natural scenes.
Karklin and Lewicki, 2009

Relationship to V1

- When trained on natural image patches
  - the dictionary columns ("atoms") look like edge detectors
  - each atom is tuned to a particular position, orientation and spatial frequency
  - V1 neurons in the mammalian brain have a similar behavior

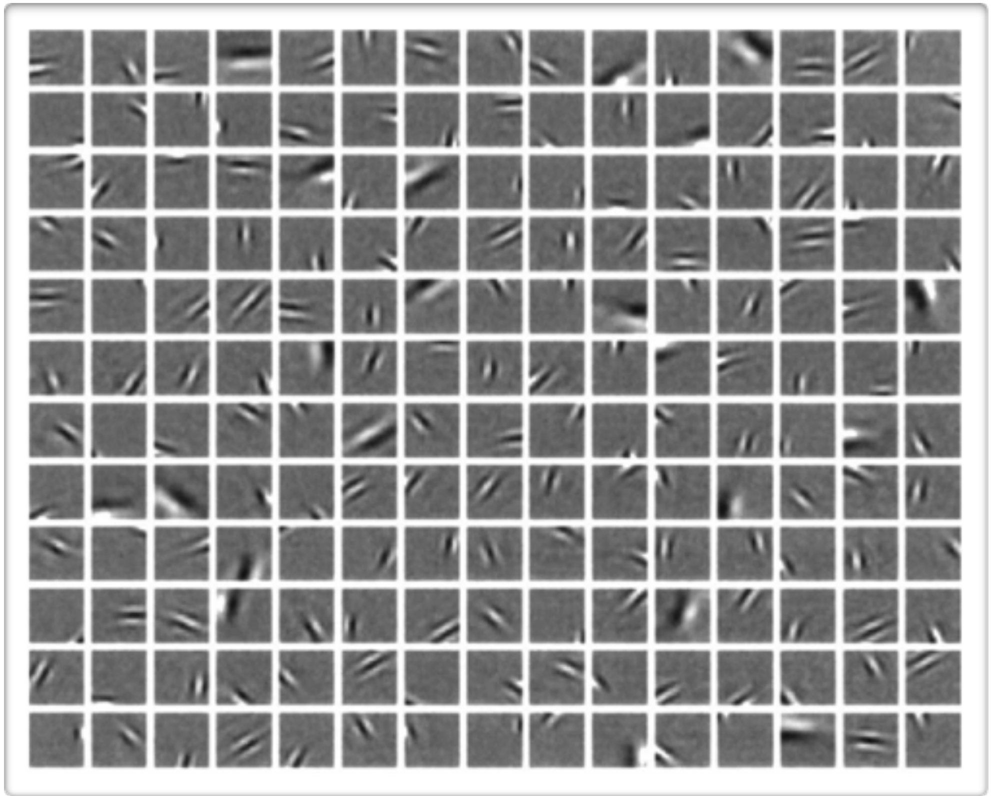


Emergence of simple-cell receptive field properties by learning a sparse code of natural images.Olshausen and Field, 1996.

Relationship to V1

• Suggests that the brain might be learning a sparse code of visual stimulus

- ➢ Since then, many other models have been shown to learn similar features
- ➢ they usually all incorporate a notion of sparsity



Emergence of simple-cell receptive field properties by learning a sparse code of natural images.Olshausen and Field, 1996.