

10417-617
Deep Learning: Fall 2020

Andrej Risteski

Machine Learning Department

Lecture 15:
Simplest of representation learners:
autoencoders and sparse coding

Unsupervised learning

Learning from data **without** labels.

What can we hope to do:

Task A: Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace, manifold) to data to reveal something meaningful about data. (**Structure learning**)

Task B: Learn a (parametrized) **distribution** *close* to data generating distribution. (**Distribution learning**)

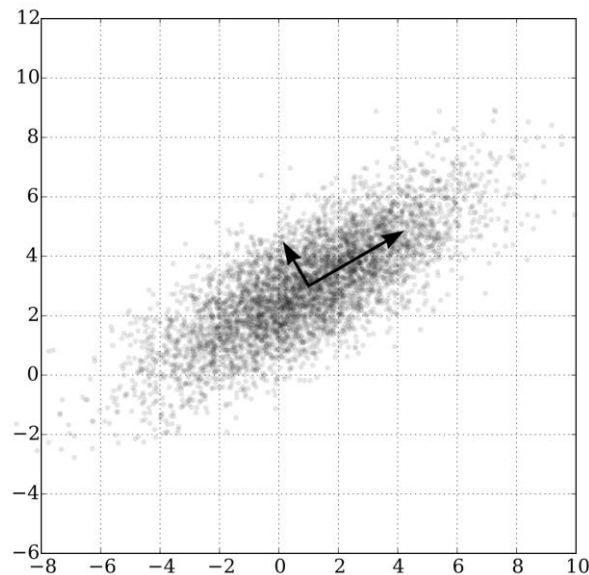
Task C: Learn a (parametrized) distribution that implicitly reveals an **“embedding”/“representation”** of data for downstream tasks. (**Representation/feature learning**)

Entangled! The “structure” and “distribution” often reveals an embedding.

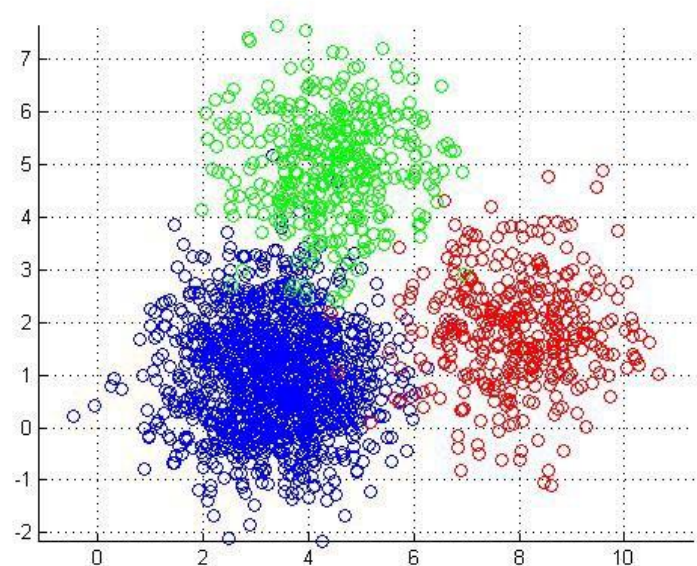
Structure learning

Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace) to data to reveal something meaningful about data.

PCA(principal component analysis),
direction of highest variance



Clustering



The simplest of representation learners

Sparse coding: learn features, s.t. each input can be written as a *sparse linear combination* of some of these features.

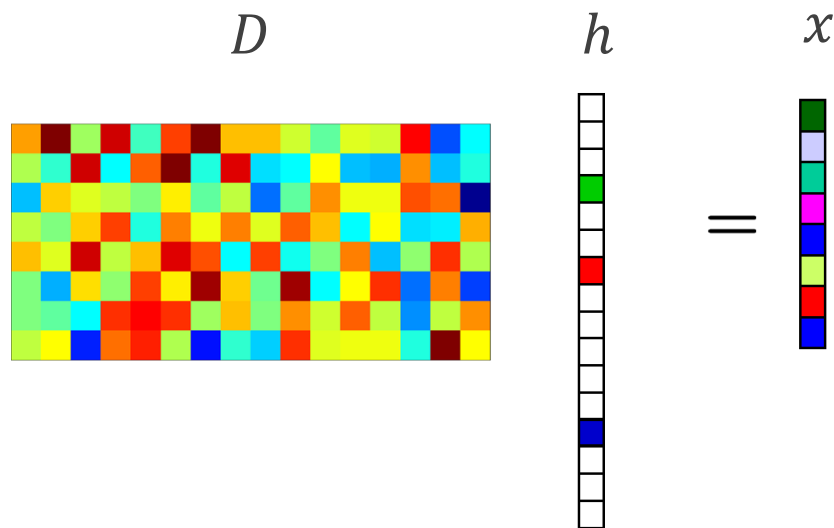
Originally made famous by *Olshausen and Field*, '96 as a model for how early visual processing works (edge detection etc.)

Autoencoders: learn encoding with some constraints (e.g. functional form, sparsity, denoising ability) from which the inputs can be approximately reconstructed.

Sparse coding

Goal: learn a *dictionary* D of features, s.t. each sample x is (approximately) writeable as a *sparse* (i.e. mostly zeros) linear combination of these features.

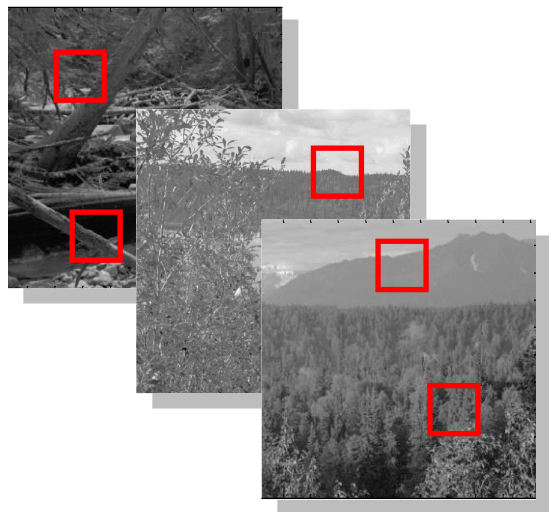
$$\forall x: \quad x \approx Dh, \quad ||h||_0 \text{ small}$$



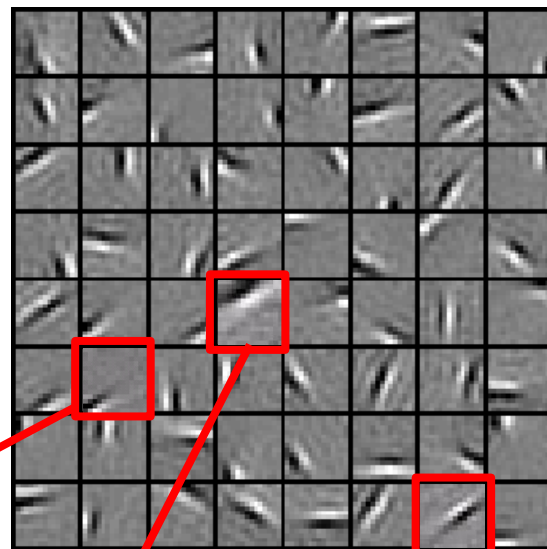
h is the representation of sample x

Sparse coding

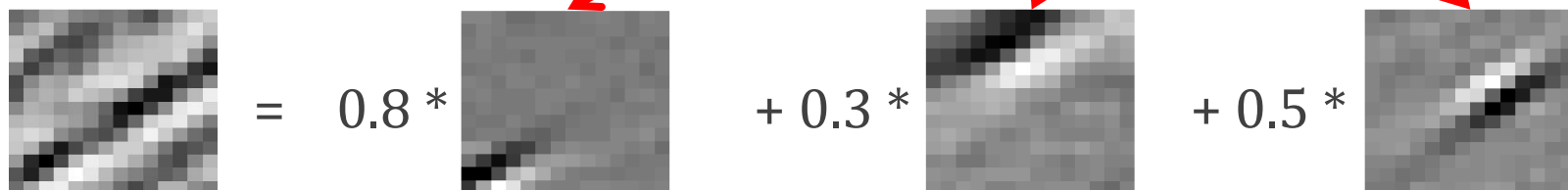
Natural Images



Learned bases: “Edges”



New example

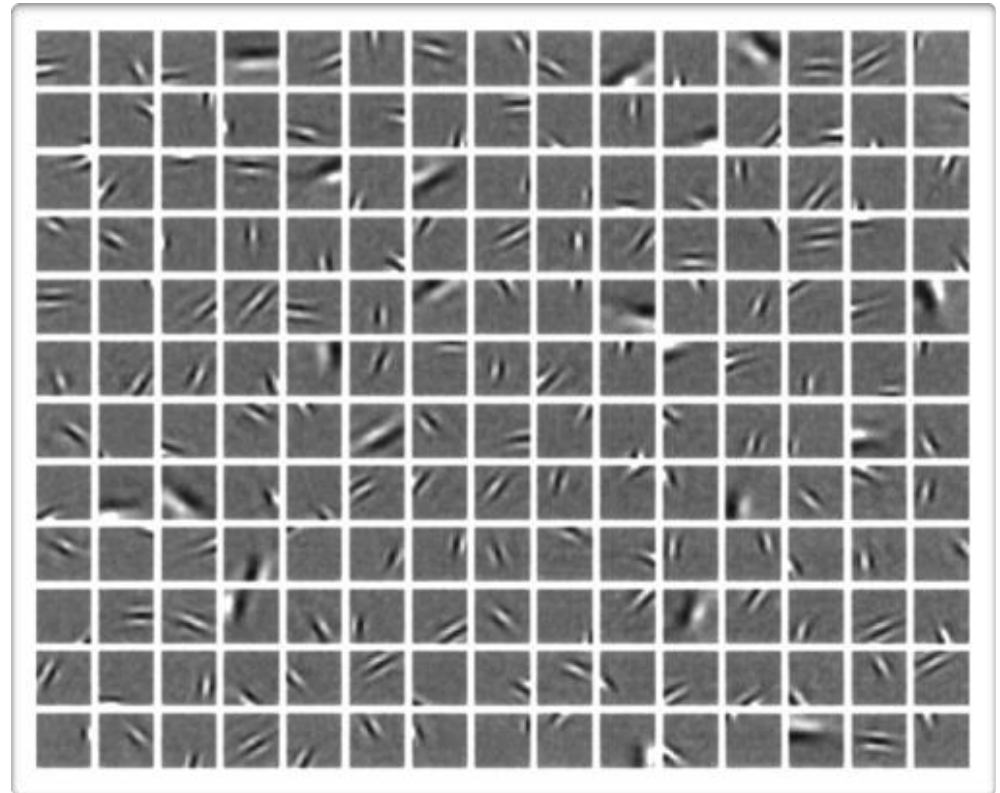


$[0, 0, \dots, 0.8, \dots, 0.3, \dots, 0.5, \dots]$ = coefficients (feature representation)

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.

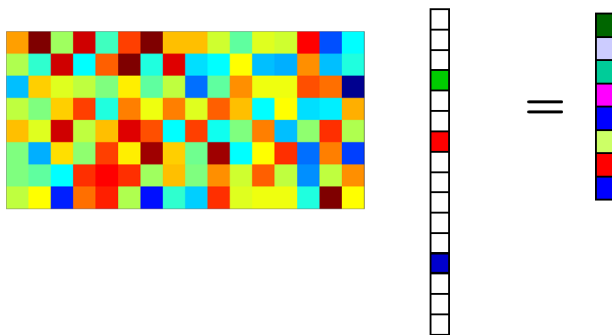
Sparse coding

Historical motivation: in signal processing, it's common to have a *fixed* dictionary D (typically, these are Fourier-basis inspired features), that's hand-crafted for the domain.

Why is this useful?: think of x as an image. It takes a lot of bits of information to write down x in the standard basis (exponential in size)

Wasteful: most vectors of numbers of image dimensions are not “real images”. There ought to be better bases... (Fourier, wavelet, ...)

In the right basis, image ought to be writeable as a combination of a *small (i.e. sparse) combination* of elements. Need much less bits to represent image ($\sim k \log d$, since there are d^k possible supports)



Sparse coding

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Sparse coding is compressive sensing, where we are learning the dictionary as well. (Fits spirit of deep learning!)

Algorithms

How do we fit \mathbf{D} ?

Obvious first try:

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^T \min_{\mathbf{h}^{(t)}} \underbrace{\frac{1}{2} \|\mathbf{x}^{(t)} - \mathbf{D} \mathbf{h}^{(t)}\|_2^2}_{\text{Reconstruction error}} + \underbrace{\lambda \|\mathbf{h}^{(t)}\|_0}_{\text{Sparsity penalty}}$$

Reconstruction: $\hat{\mathbf{x}}^{(t)}$ Sparsity vs. reconstruction control

Can't quite take gradients: l_0 is either flat (gradients are 0) or not differentiable.

Algorithms

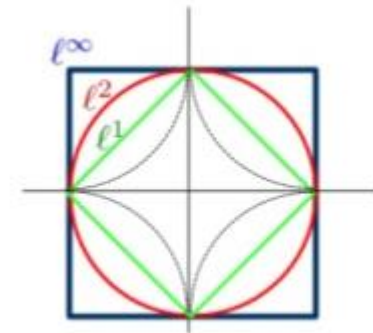
How do we fit \mathbf{D} ?

Typical relaxation:

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

Reconstruction: $\hat{\mathbf{x}}^{(t)}$ Sparsity vs. reconstruction control

l_1 is the convex envelope of l_0 : the closest function that is convex.



Algorithms

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Reconstruction: $\hat{\mathbf{x}}^{(t)}$ (indicated by a red arrow pointing to $\mathbf{x}^{(t)}$)

Sparsity vs. reconstruction control (indicated by a red arrow pointing to λ)

- ⌘ We also constrain the columns of D to be of norm 1
- ⌘ Otherwise, we can **scale D up, scale h's down**, which improves sparsity penalty, but clearly doesn't encourage sparsity.

Inference

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

- ⌘ We need to optimize:

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

- ⌘ *Usual candidate:* gradient descent

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

- ⌘ *Issue:* l_1 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, clamp to 0.

- ⌘ Sometimes called **ISTA (Iterative Shrinkage Thresholding Algorithm)**

Inference

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

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

Each hidden unit update would be performed as follows:

- ⊗ $h_k^{(t)} \Leftarrow h_k^{(t)} - \alpha (\mathbf{D}_{\cdot,k})^\top (\mathbf{D} \mathbf{h}^{(t)} - \mathbf{x}^{(t)})$

Update from
reconstruction

- ⊗ If $\text{sign}(h_k^{(t)}) \neq \text{sign}(h_k^{(t)} - \alpha \lambda \text{sign}(h_k^{(t)}))$ then $h_k^{(t)} \Leftarrow 0$

- ⊗ Else $h_k^{(t)} \Leftarrow h_k^{(t)} - \alpha \lambda \text{sign}(h_k^{(t)})$

Update sparsity
term

Inference: some intuition

Let's assume that $x = Dh^* + \epsilon$, for an orthogonal D ($D^T D = I$), s.t. $\|\epsilon\|_2 \leq \frac{\tau}{4}$.
Let's assume h^* is *sparse* and the non-zero entries satisfy $|h_i^*| \geq \tau$ if $h_i^* \neq 0$.

The ISTA update looks like: $h \leftarrow h - \alpha(D^T(Dh - x))$

$$\text{If } \text{sgn}(h_k) \neq \text{sgn}(h_k - \alpha\lambda \text{sgn}(h_k)) \Rightarrow h_k \leftarrow 0$$

Set $\alpha = 1, \lambda = \tau/2$. Then, we have: $h \leftarrow D^T x = D^T(Dh^* + \epsilon) = h^* + D^T \epsilon$

Note that $\langle D_{:,k}, \epsilon \rangle \leq \|\epsilon\|_2$ by orthogonality, so $h_i = h_i^* + \delta_i, |\delta_i| \leq \frac{\tau}{4}$

$$\text{If } h_i^* \neq 0, |h_i| \geq \frac{3\tau}{4} \Rightarrow \text{sgn}(h_i) = \text{sgn}(h_i - \tau/2 \text{sgn}(h_i))$$

$$\text{If } h_i^* \neq 0, |h_i| \leq \frac{\tau}{4} \Rightarrow \text{sgn}(h_i) \neq \text{sgn}(h_i - \tau/2 \text{sgn}(h_i))$$

*We are done in
one step!*

Note: when done, we get the support of h^* right (i.e. $h_i \neq 0$ if and only if $h_i^* \neq 0$)
The sgn step is a great denoiser! It (correctly) sets to 0 small coordinates of h_i .
Since h^* is *sparse* this is in fact most of the coordinates!

Dictionary learning algorithm

Given that we have a mechanism for finding good \mathbf{h} 's for a fixed dictionary, we can do the same thing we did in the EM algorithm: alternate optimizing.

Keeping the \mathbf{h} 's fixed, perform gradient descent for \mathbf{D} :

- Perform gradient update of \mathbf{D}

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

- Renormalize the columns of \mathbf{D}
- For each column of \mathbf{D} :

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

Dictionary learning algorithm

Given that we have a mechanism for finding good \mathbf{h} 's for a fixed dictionary, we can do the same thing we did in the EM algorithm: alternate optimizing.

While \mathbf{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 by running gradient descent for \mathbf{D} .

Some applications

tie					spring				
trousers	season	scoreline	wires	operatic	beginning	dampers	flower	creek	humid
blouse	teams	goalless	cables	soprano	until	brakes	flowers	brook	winters
waistcoat	winning	equaliser	wiring	mezzo	months	suspension	flowering	river	summers
skirt	league	clinchng	electrical	contralto	earlier	absorbers	fragrant	fork	ppen
sleeved	finished	scoreless	wire	baritone	year	wheels	lilies	piney	warm
pants	championship	replay	cable	coloratura	last	damper	flowered	elk	temperatures

Table 6: Five discourse atoms linked to the words *tie* and *spring*. Each atom is represented by its nearest 6 words. The algorithm often makes a mistake in the last atom (or two), as happened here.

Finding the different meanings of polysemous words
(Arora, Li, Liang, Ma, Risteski '18)

Some applications

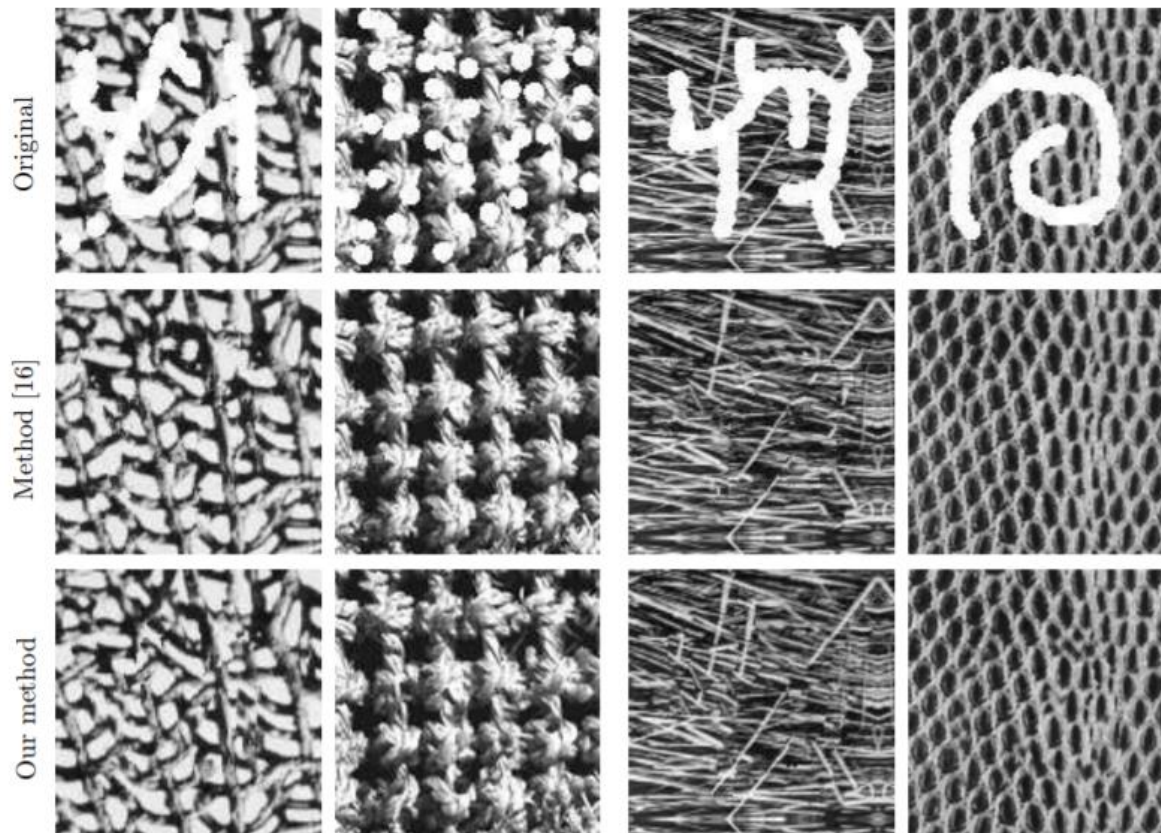
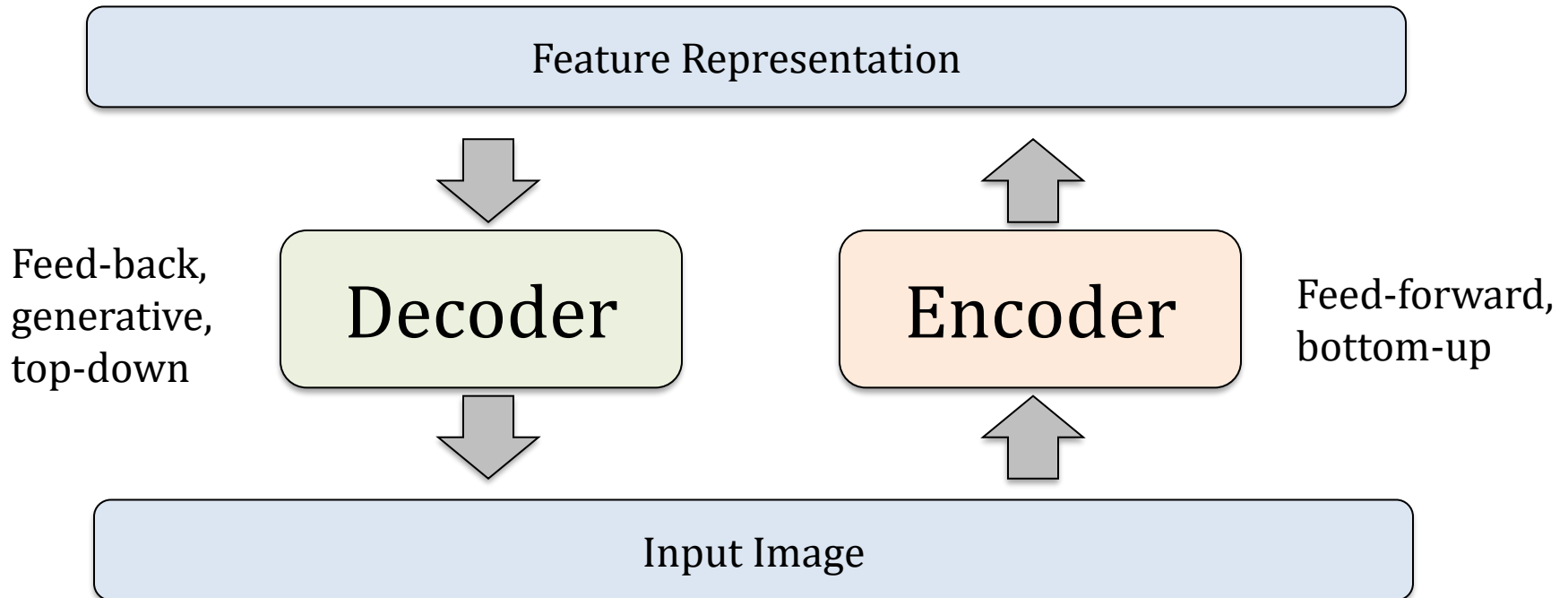


Figure 8: *Examples of inpainting using [16] and using the proposed method.*

Sparse Modeling of Textures
(Gabriel Peyré, '09)

Autoencoders

The idea behind autoencoders: learn features, s.t. input is reconstructable from them

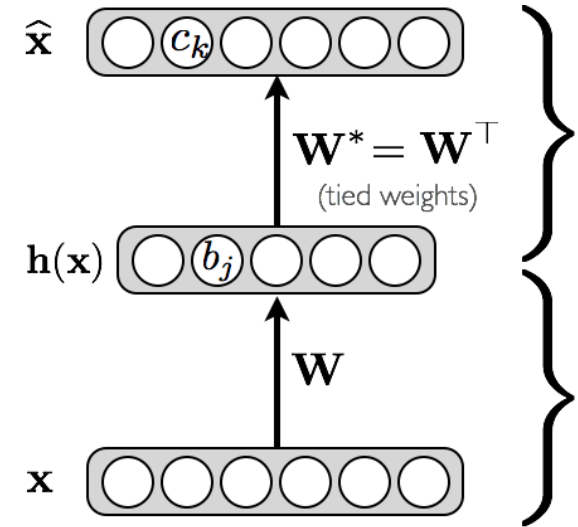


- Details of what goes inside the encoder and decoder matter!
 - Need *constraints* to **avoid learning an identity**.

Autoencoders

Some way to prevent identity:

- *Weight tying* of encoder/decoder. (Often magical!)
- *Smaller dimension* for latent variables
- Enforce *sparsity* of the latent representation
- Encourage decoder to be robust to adding noise to \mathbf{x} . (*Denoising autoencoder*)
- Encode to distribution rather than pointmass. (*Variational autoencoder*)



Typical losses

Loss function for inputs between 0 and 1

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

⊗ *Cross-entropy error* ($f(\mathbf{x}) \equiv \hat{\mathbf{x}}$)

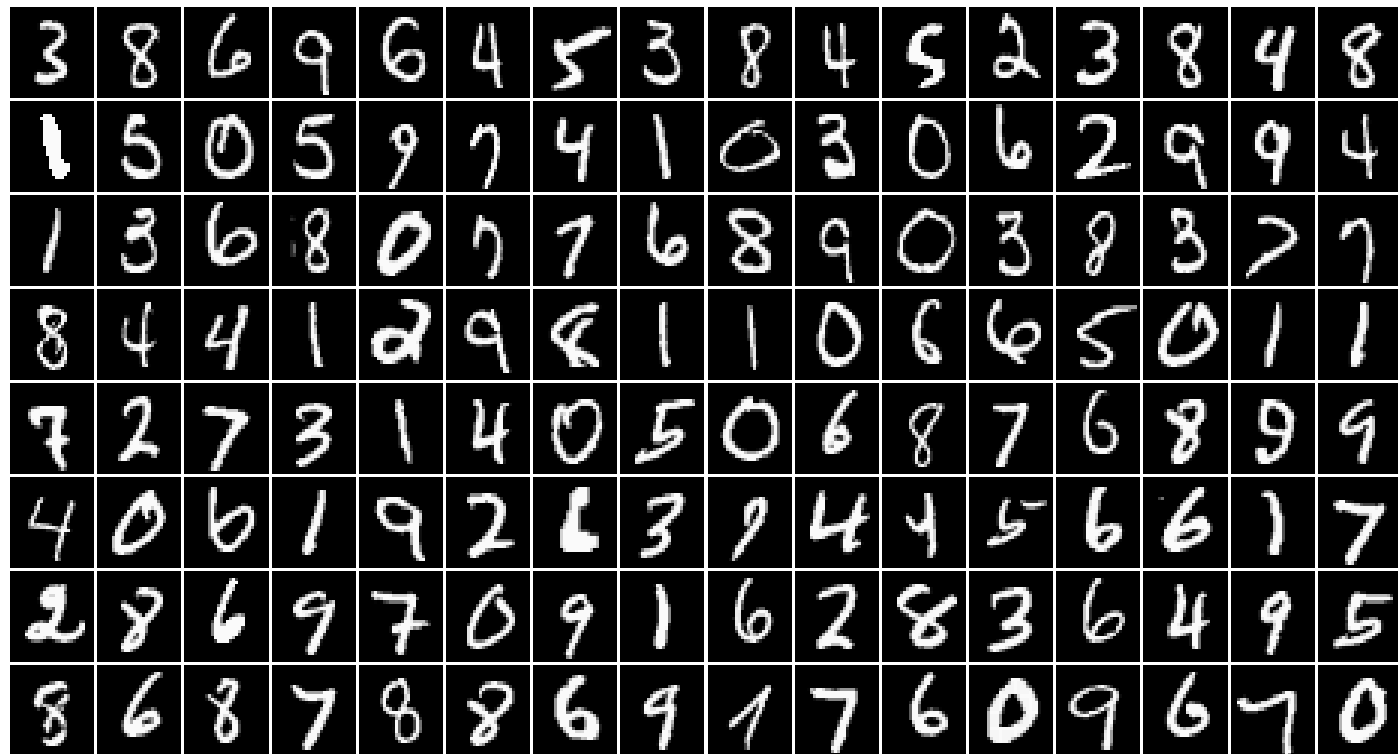
Loss function for real-valued inputs

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

⊗ l_2 error

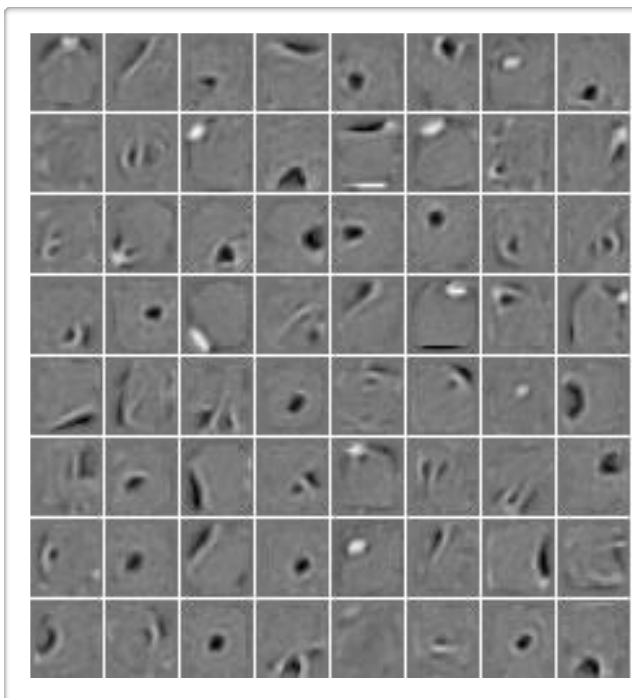
⊗ we use a linear activation function at the output

Example: Reconstructions on MNIST

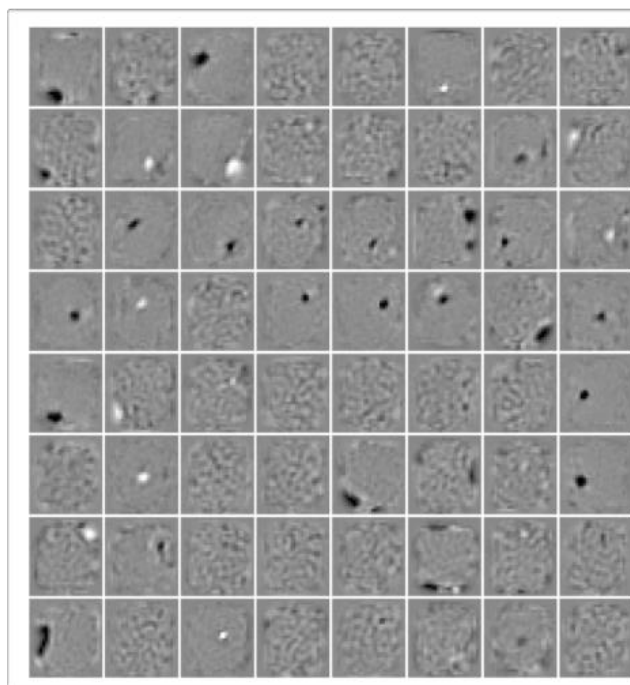


Learned Features

MNIST dataset:

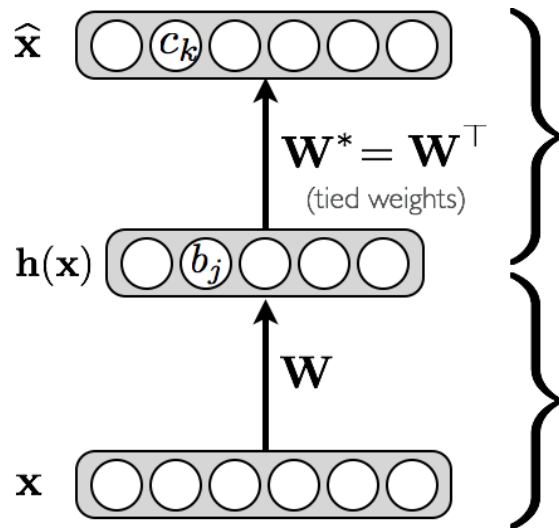


RBM



Autoencoder

Intuitions for weight tying



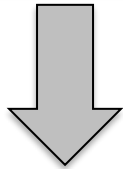
Original intuition: similar as doing 2 steps in a Gibbs sampler in RBM's.
(Though not randomized.)

Better intuition: one step of ISTA algorithm for dictionary learning!

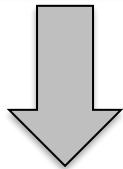
Intuitions for weight tying

Setup: sgn activations with weight tying

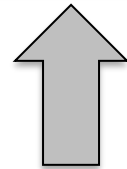
Features $z \in \{0, \pm\tau\}^d$



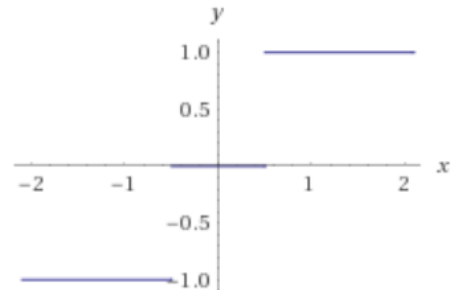
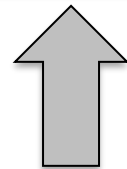
Wz



Input Image x



$z = \tau \text{thr}_{\tau/2}(W^T x)$



Intuitions for weight tying

Claim: if true x 's satisfy $x = Wz + \epsilon$, for W orthogonal, $\|\epsilon\|_2 \leq \frac{\tau}{4}$, the above combination of encoder/decoders give a reconstruction error of at most $\|\epsilon\|_2$

Same calculation as doing one ISTA step!

Encoder produces: $\text{thr}_{\tau/2}(W^T x) = \text{thr}_{\tau/2}(W^T(Wz + \epsilon))$
 $= \text{thr}_{\tau/2}(z + W^T \epsilon)$

As $\langle W_{:,k}, \epsilon \rangle \leq \|\epsilon\|_2$, encoder produces $z_i + \delta_i$, $|\delta_i| \leq \frac{\tau}{4}$.

If $|z_i| = \tau$, input to thr is $z_i + \delta_i \in \tau \pm \frac{\tau}{4}$, hence encoder produces z_i

If $z_i = 0$, input to thr is $z_i + \delta_i \in \pm \frac{\tau}{4}$, hence encoder produces 0.

Hence, correct z is recovered!

Also, $\|\hat{x} - x\|_2 = \|Wz - x\|_2 = \|\epsilon\|_2$, which is small!

Variants, variants, variants

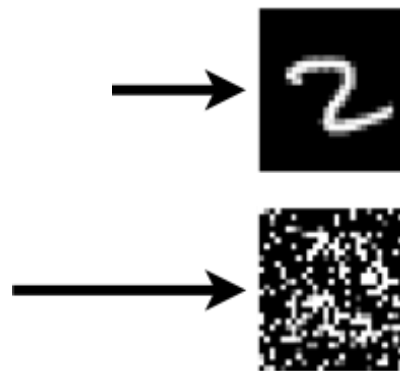
Undercomplete Representation

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 (*maybe not even*)

Hidden units will be

- good features for the training distribution (*potentially...*)
- will not be robust to other types of input (*not trained to compress these*)



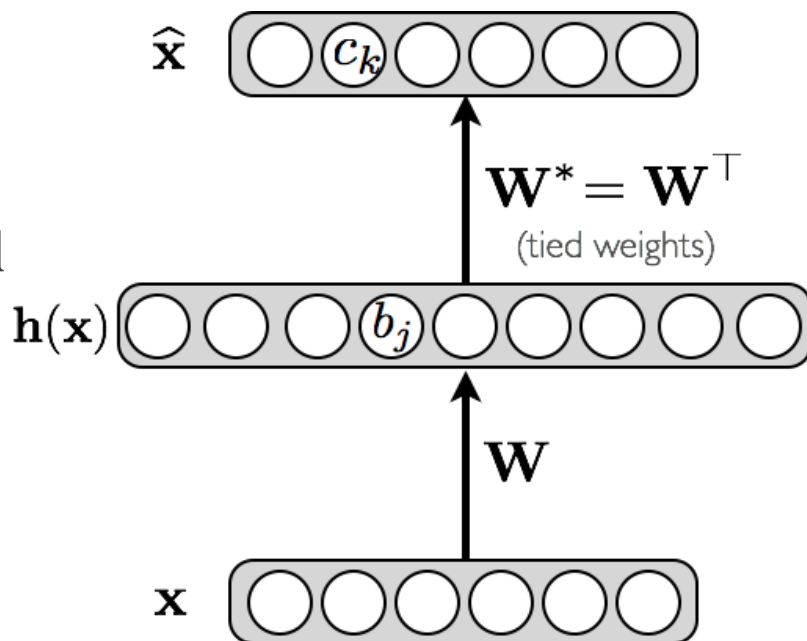
Overcomplete Representation

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

Other constraints must be made, e.g. *sparsity*, *denoising*, etc.

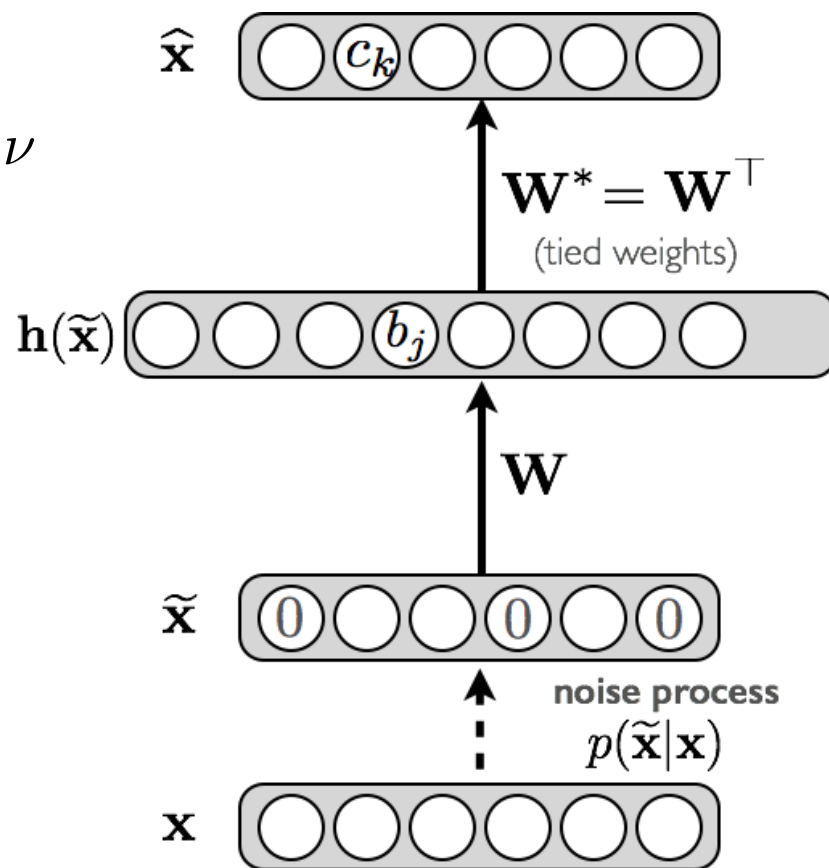


Denoising Autoencoder

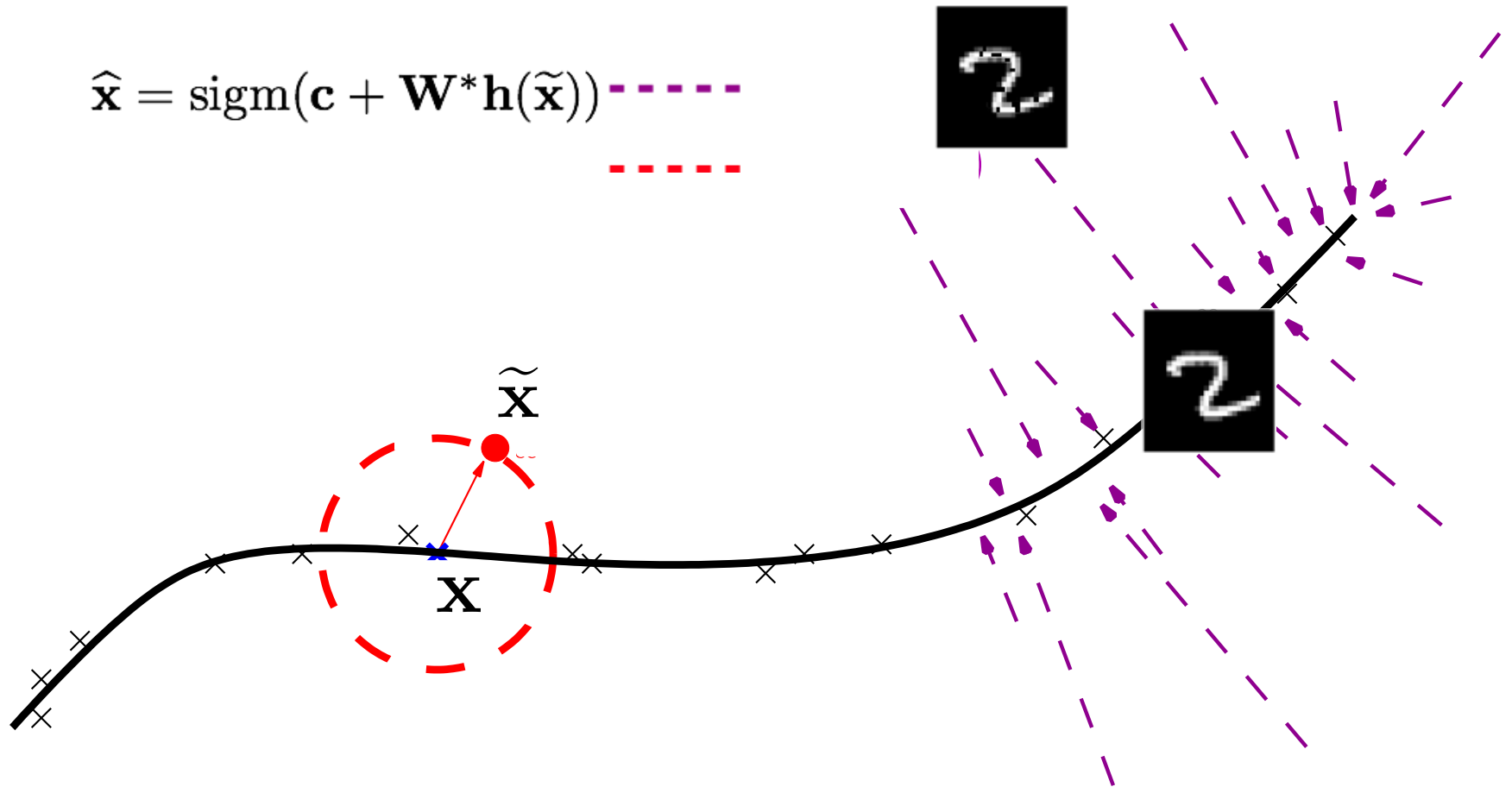
Idea: representation should be *robust to introduction of noise*:

- *Dropout*: random assignment of subset of inputs to 0, with probability ν
- *Gaussian additive noise*

- Reconstruction $\hat{\mathbf{x}}$ computed from the corrupted input $\tilde{\mathbf{x}}$
- Loss function compares $\hat{\mathbf{x}}$ reconstruction with the noiseless input \mathbf{x}

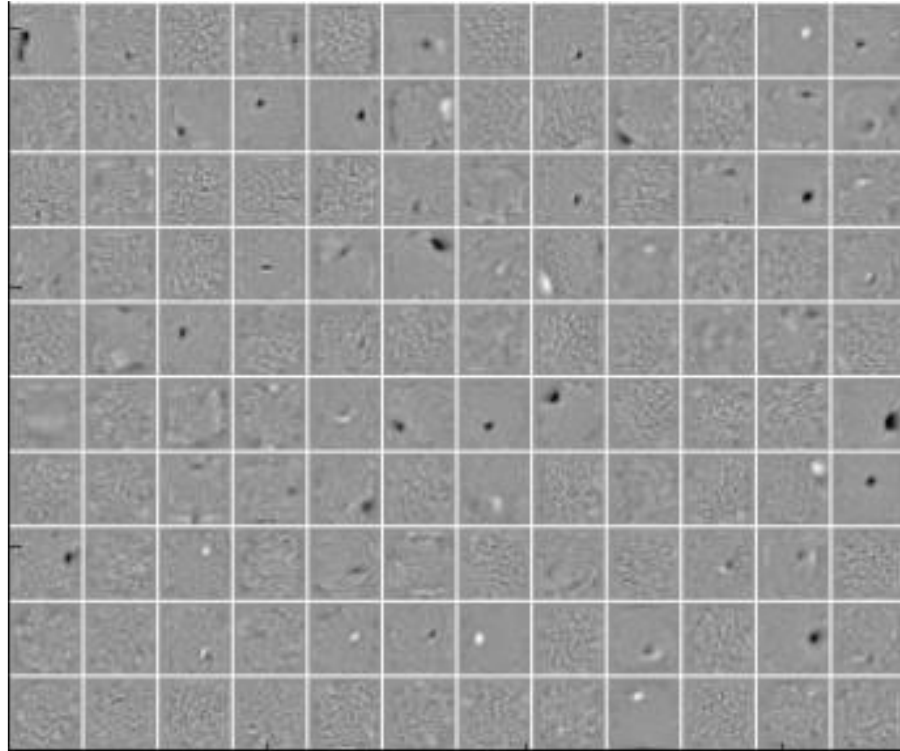


Denoising Autoencoder

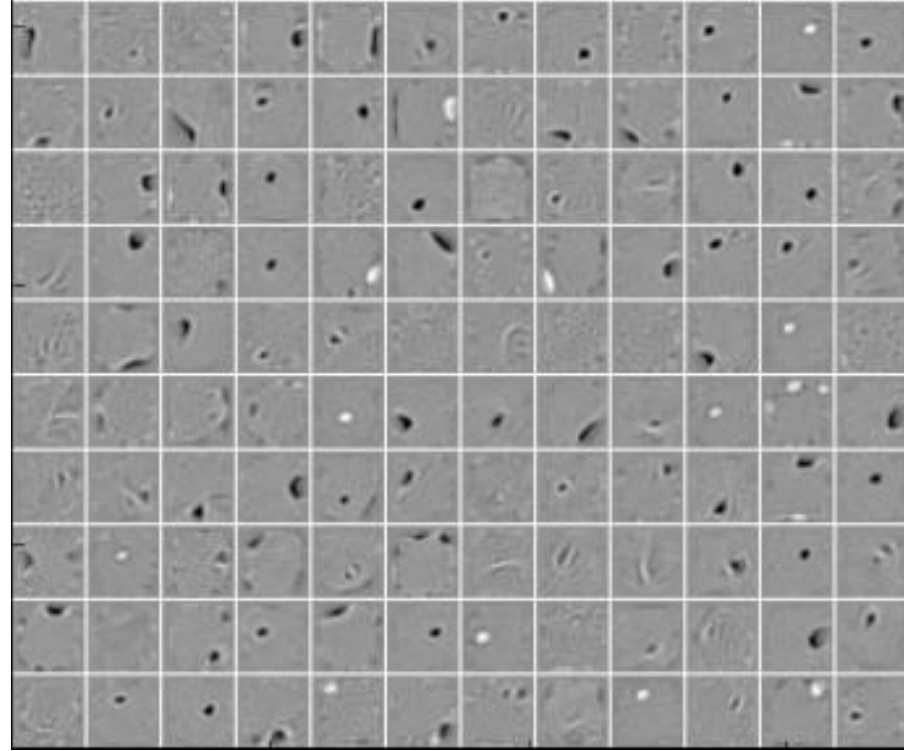


Learned Filters

Non-corrupted

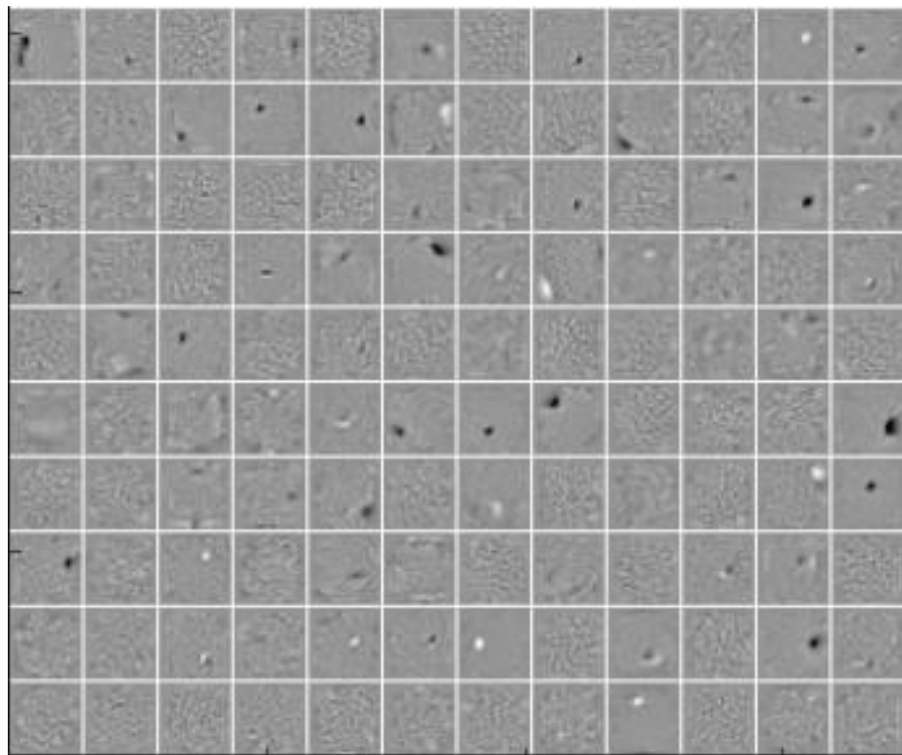


25% corrupted input

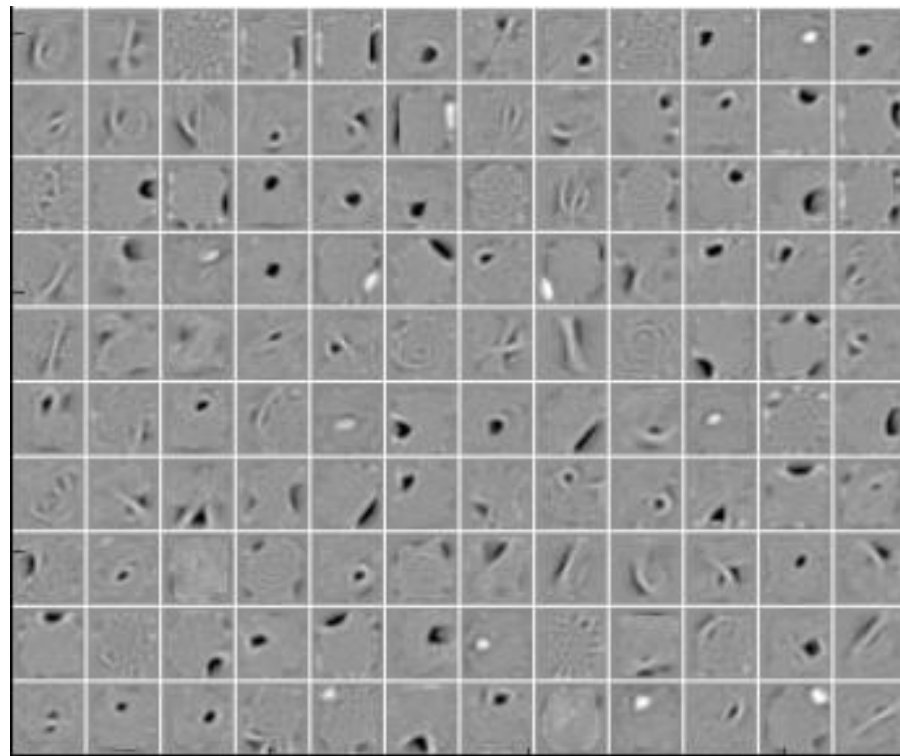


Learned Filters

Non-corrupted



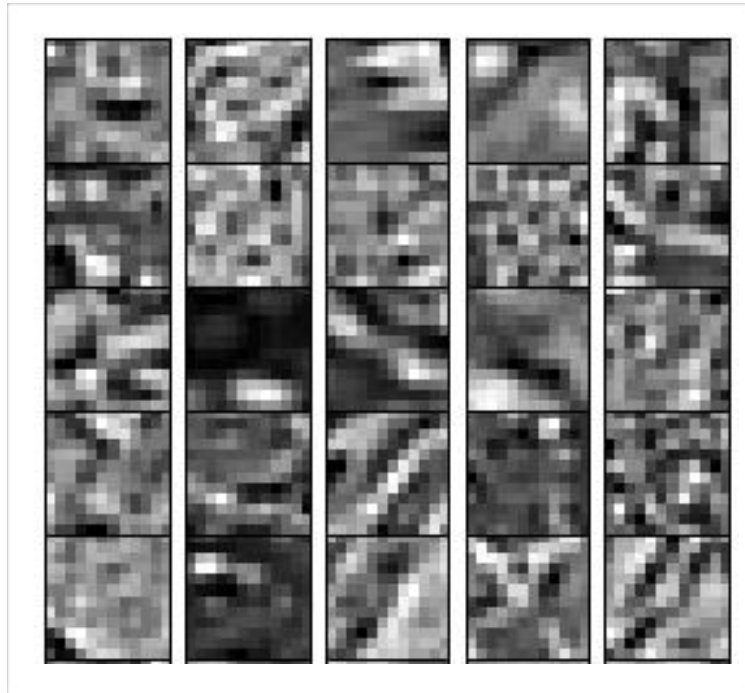
50% corrupted input



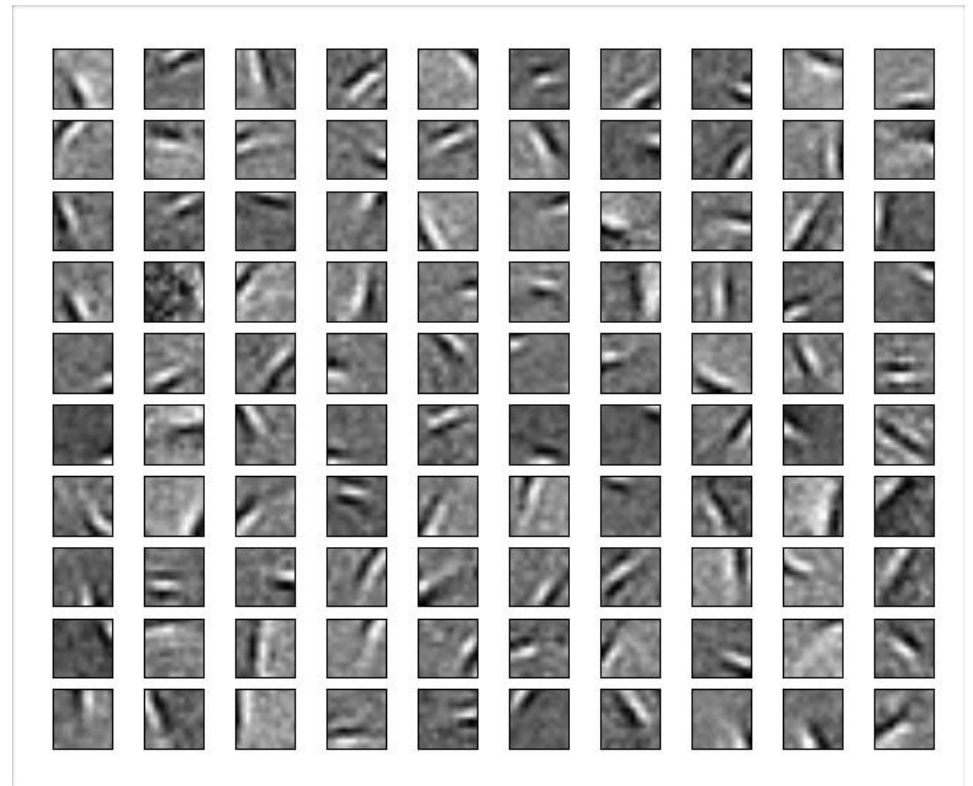
Squared Error Loss

Training on natural image patches, with squared loss

PCA may not be the best solution

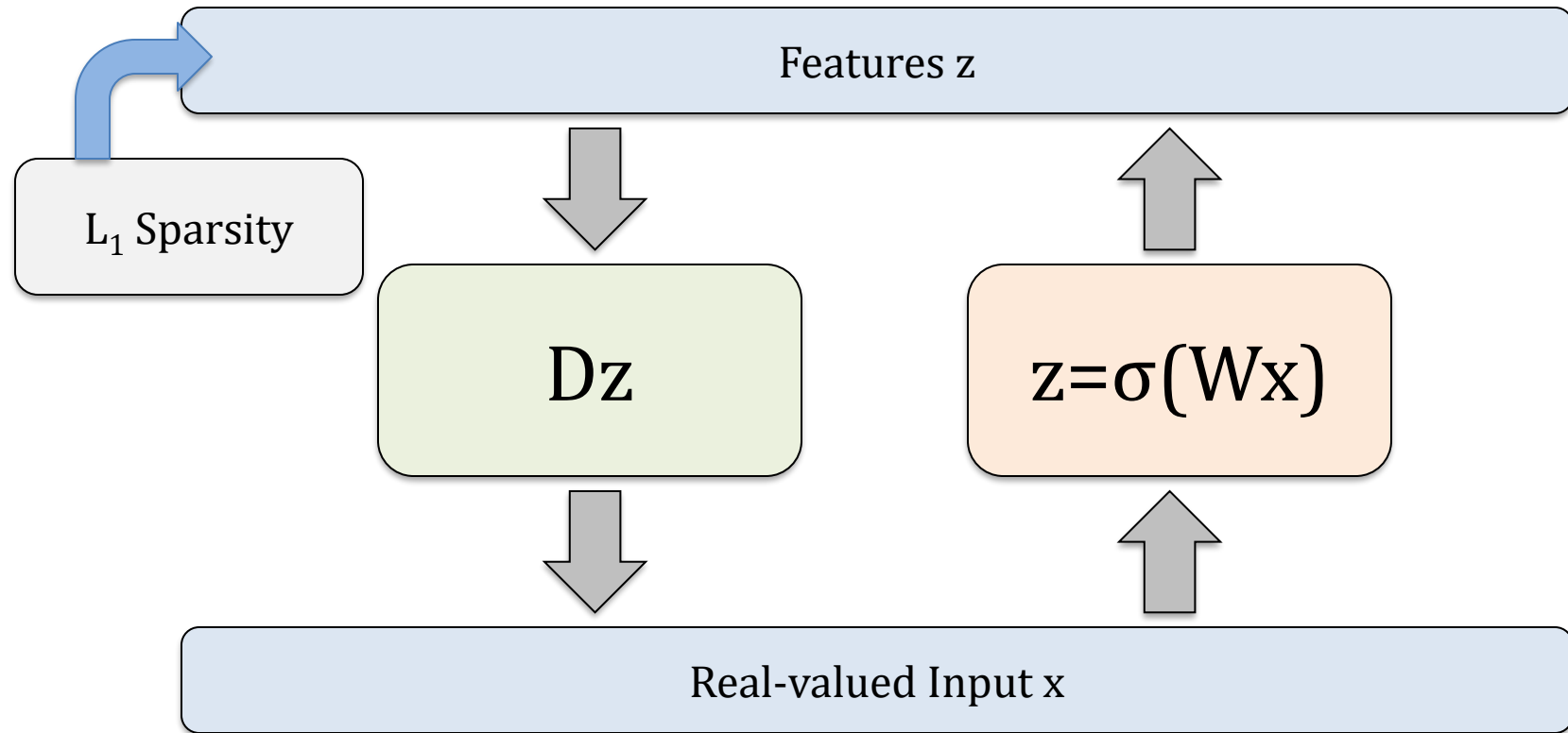


Data



Filters

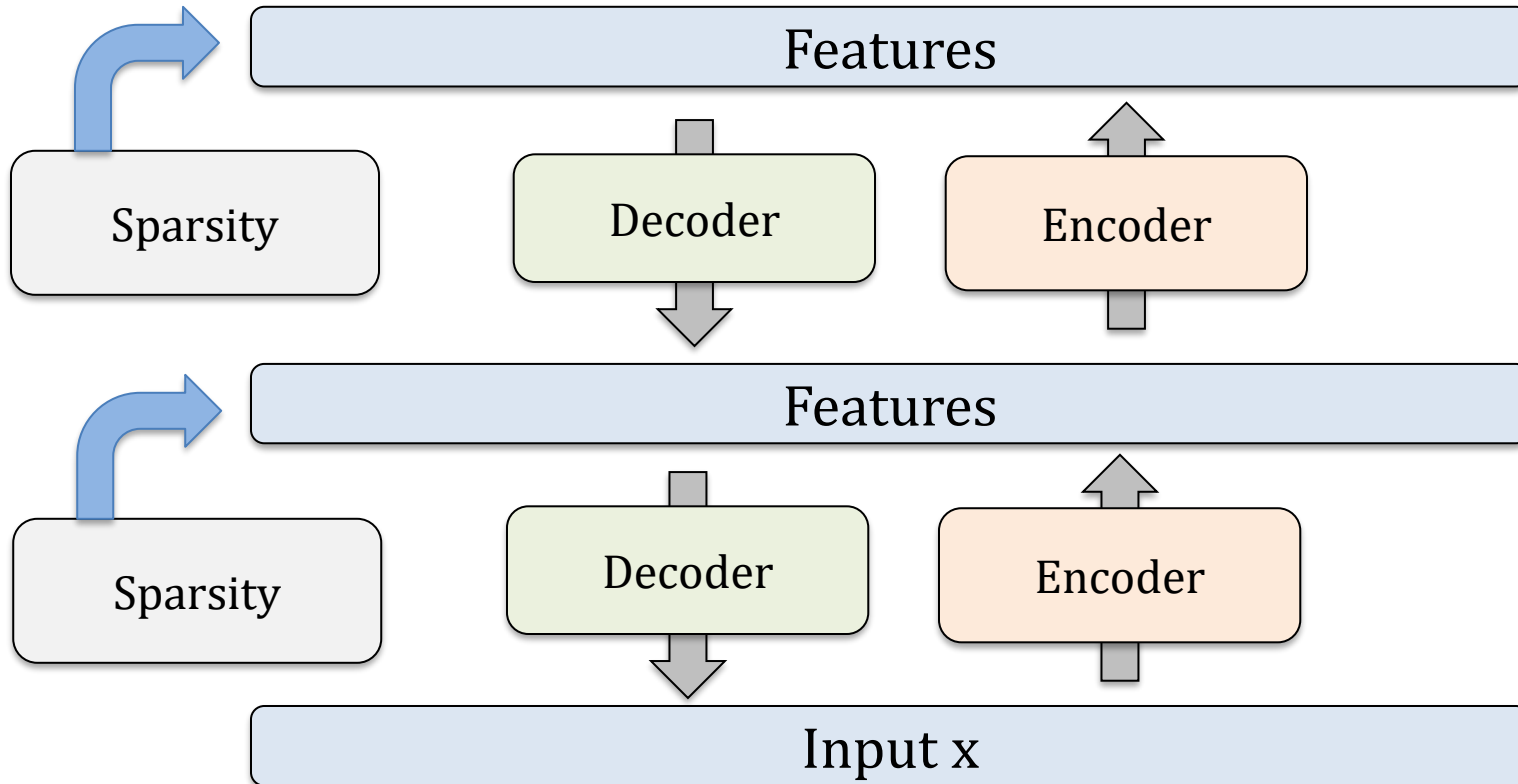
Sparsity



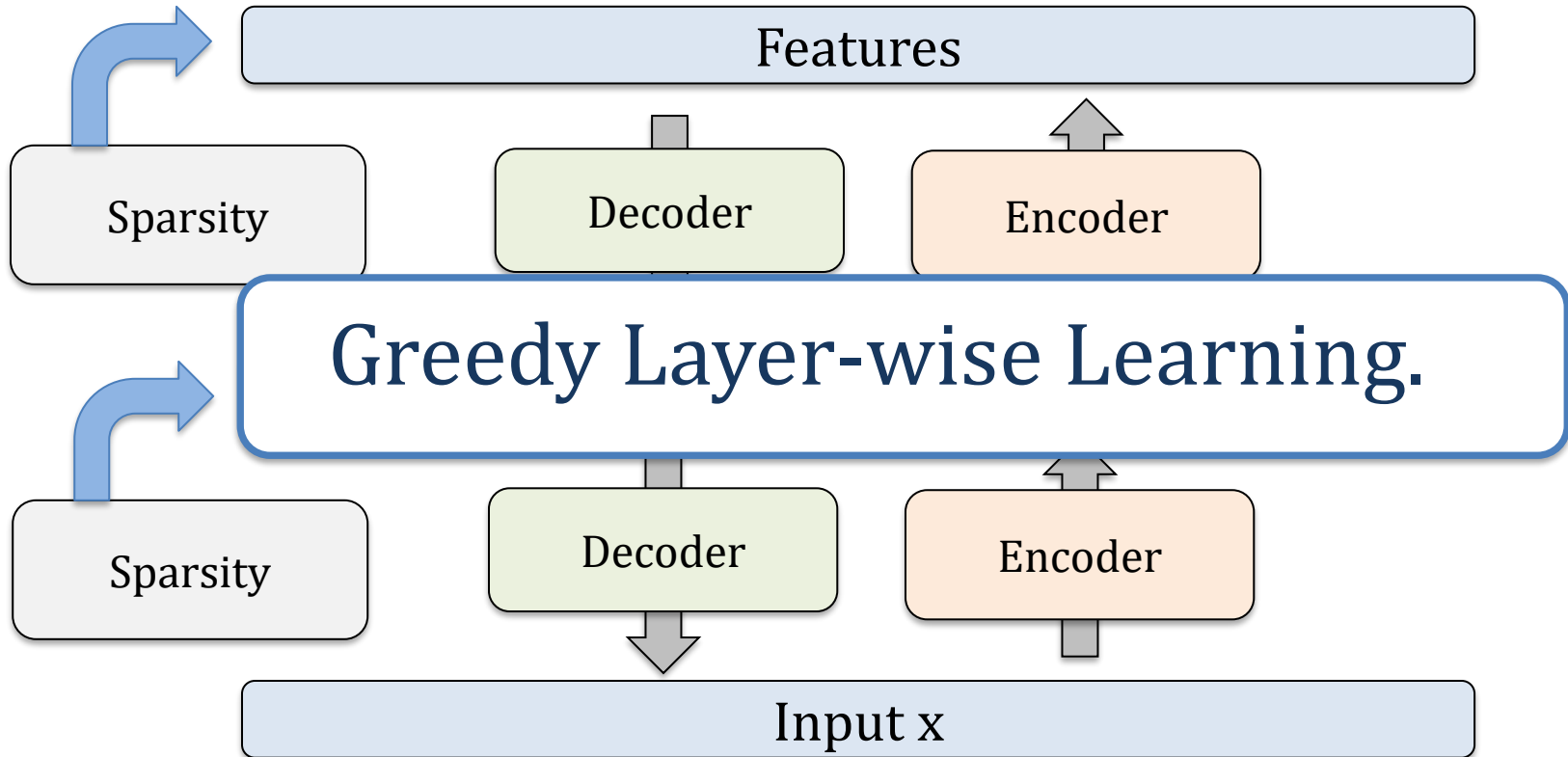
At training
time

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

Stacked Autoencoders



Stacked Autoencoders



Parameters can be fine-tuned using backpropagation.

Deep Autoencoders

Some sample reconstructions:



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