Neural networks

Sparse coding - definition

UNSUPERVISED LEARNING

Topics: unsupervised learning

- Unsupervised learning: 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 trainings

- We will see 3 neural networks for unsupervised learning
  - restricted Boltzmann machines
  - autoencoders
  - **sparse coding model**

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

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

  - we also constrain the columns of $\mathbf{D}$ to be of norm 1
    - otherwise, $\mathbf{D}$ could grow big while $\mathbf{h}^{(t)}$ becomes small to satisfy the prior
  - sometimes the columns are constrained to be no greater than 1

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

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

  - we also constrain the columns of $\mathbf{D}$ to be of norm 1
    - otherwise, $\mathbf{D}$ could grow big while $\mathbf{h}^{(t)}$ becomes small to satisfy the prior
  - sometimes the columns are constrained to be no greater than 1

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

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

  - we also constrain the columns of $\mathbf{D}$ to be of norm 1
    - otherwise, $\mathbf{D}$ could grow big while $\mathbf{h}^{(t)}$ becomes small to satisfy the prior
  - sometimes the columns are constrained to be no greater than 1

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

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

  - we also constrain the columns of $\mathbf{D}$ to be of norm 1
    - otherwise, $\mathbf{D}$ could grow big while $\mathbf{h}^{(t)}$ becomes small to satisfy the prior
  - sometimes the columns are constrained to be no greater than 1

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} \overbrace{||\mathbf{x}^{(t)} - \underbrace{\mathbf{D}\,\mathbf{h}^{(t)}}_{\text{reconstruction } \widehat{\mathbf{x}}^{(t)}}||_2^2}^{\text{reconstruction error}} + \underbrace{\lambda}_{\text{reconstruction vs. sparsity control}} \overbrace{||\mathbf{h}^{(t)}||_1}^{\text{sparsity penalty}}$$

  - we also constrain the columns of $\mathbf{D}$ to be of norm 1
    - otherwise, $\mathbf{D}$ could grow big while $\mathbf{h}^{(t)}$ becomes small to satisfy the prior
  - sometimes the columns are constrained to be no greater than 1

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as well as possible
- More formally:

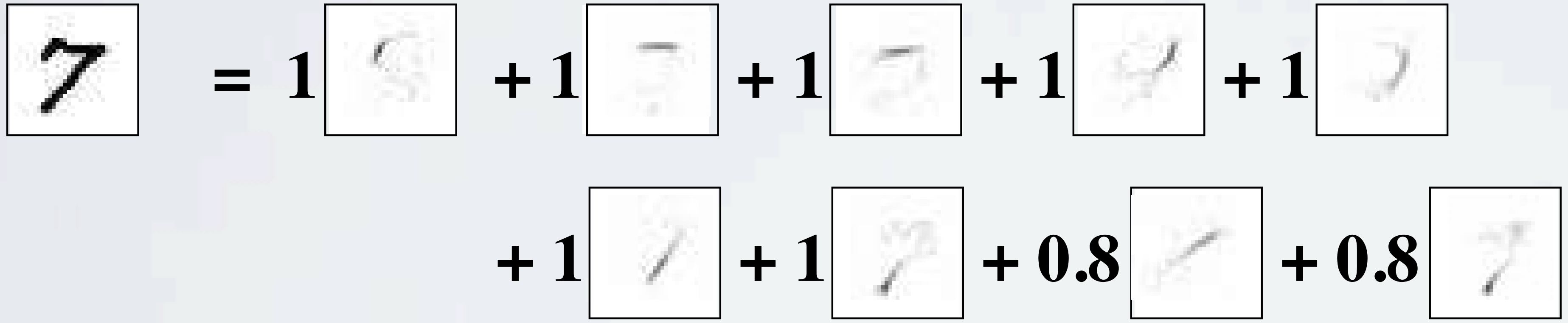
$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} \overbrace{||\mathbf{x}^{(t)} - \underbrace{\mathbf{D}\,\mathbf{h}^{(t)}}_{\text{reconstruction } \widehat{\mathbf{x}}^{(t)}}||_2^2}^{\text{reconstruction error}} + \underbrace{\lambda}_{\text{reconstruction vs. sparsity control}} \overbrace{||\mathbf{h}^{(t)}||_1}^{\text{sparsity penalty}}$$

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

SPARSE CODING

Topics: dictionary

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

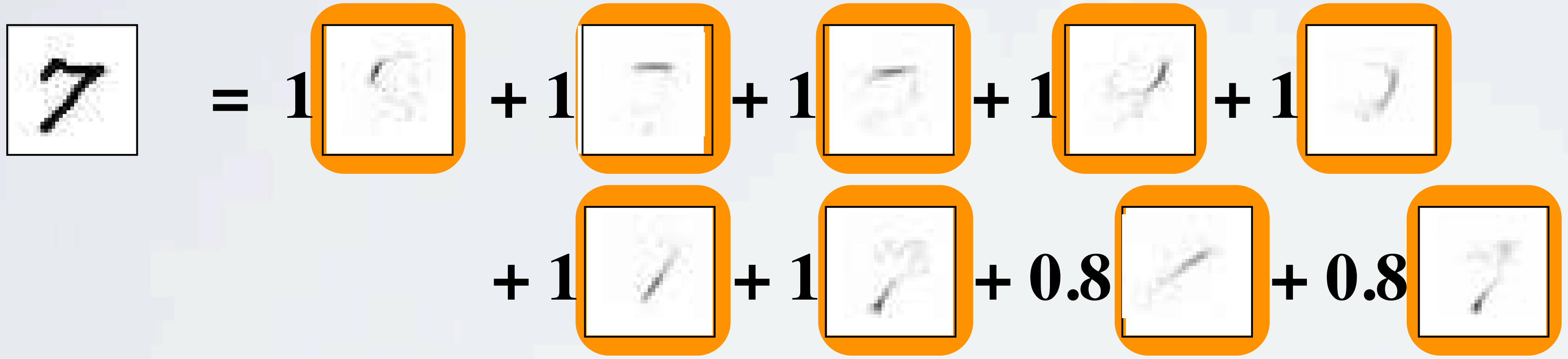


  - we also refer to $\mathbf{D}$ as the dictionary
    - in certain applications, we know what dictionary matrix to use
    - often however, we have to learn it

SPARSE CODING

Topics: dictionary

- Can also write $\widehat{\mathbf{x}}^{(t)} = \mathbf{D}\,\mathbf{h}(\mathbf{x}^{(t)}) = \sum\limits_{\substack{k \text{ s.t.} \\ h(\mathbf{x}^{(t)})_k \neq 0}} \boxed{\mathbf{D}_{\cdot,k}}\, h(\mathbf{x}^{(t)})_k$

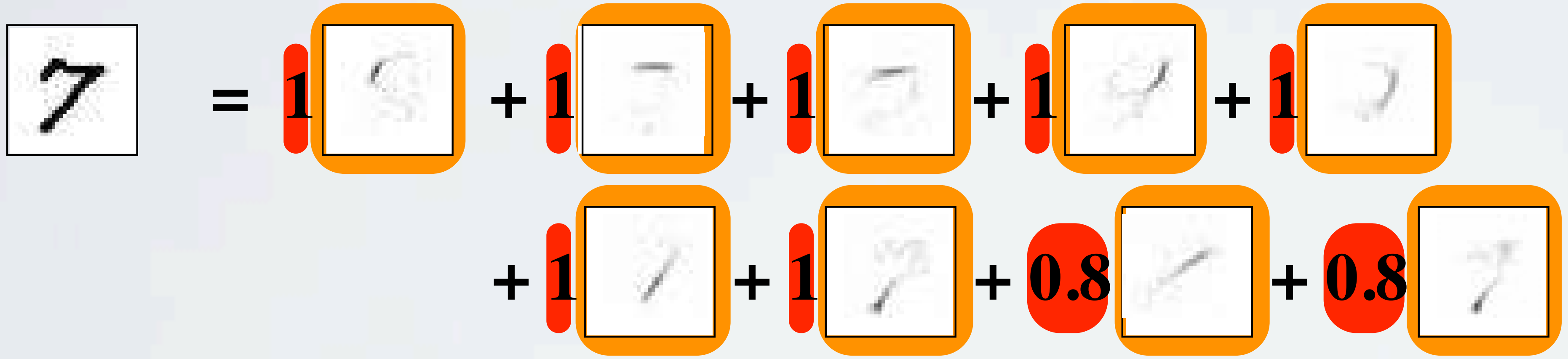


  - we also refer to $\mathbf{D}$ as the dictionary
    - in certain applications, we know what dictionary matrix to use
    - often however, we have to learn it

SPARSE CODING

Topics: dictionary

- Can also write $\widehat{\mathbf{x}}^{(t)} = \mathbf{D}\,\mathbf{h}(\mathbf{x}^{(t)}) = \sum\limits_{\substack{k \text{ s.t.} \\ h(\mathbf{x}^{(t)})_k \neq 0}} \mathbf{D}_{\cdot,k}\, h(\mathbf{x}^{(t)})_k$



  - we also refer to $\mathbf{D}$ as the dictionary
    - in certain applications, we know what dictionary matrix to use
    - often however, we have to learn it

Neural networks

Sparse coding - inference (ISTA algorithm)

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as much as possible
- More formally:

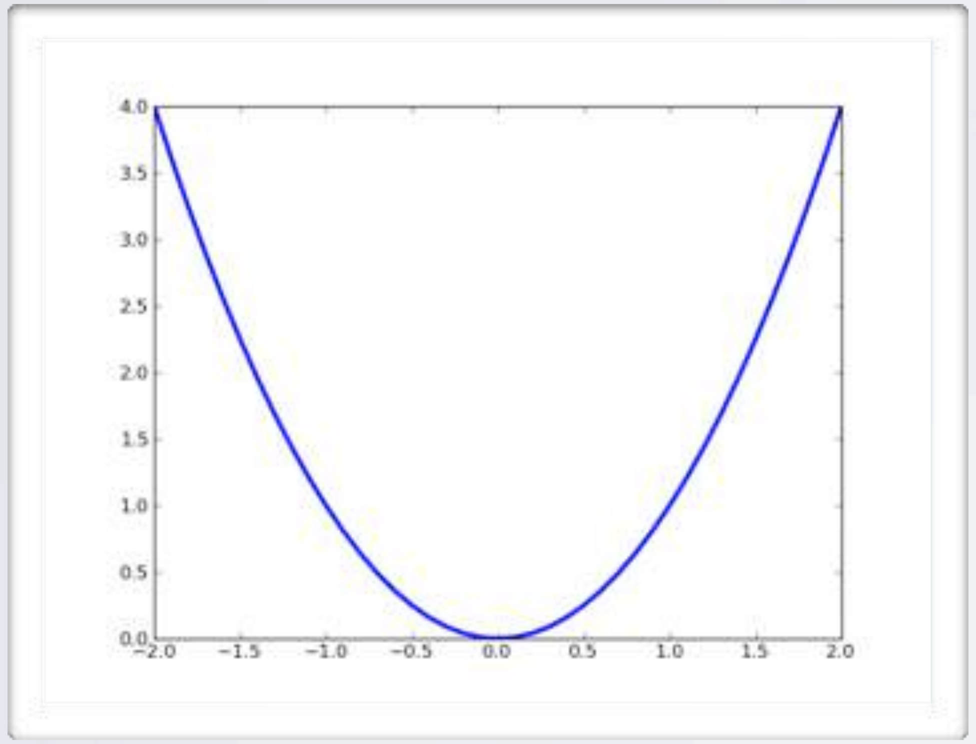
$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} \overbrace{||\mathbf{x}^{(t)} - \underbrace{\mathbf{D}\,\mathbf{h}^{(t)}}_{\text{reconstruction } \widehat{\mathbf{x}}^{(t)}}||_2^2}^{\text{reconstruction error}} + \underbrace{\lambda}_{\text{reconstruction vs. sparsity control}} \overbrace{||\mathbf{h}^{(t)}||_1}^{\text{sparsity penalty}}$$

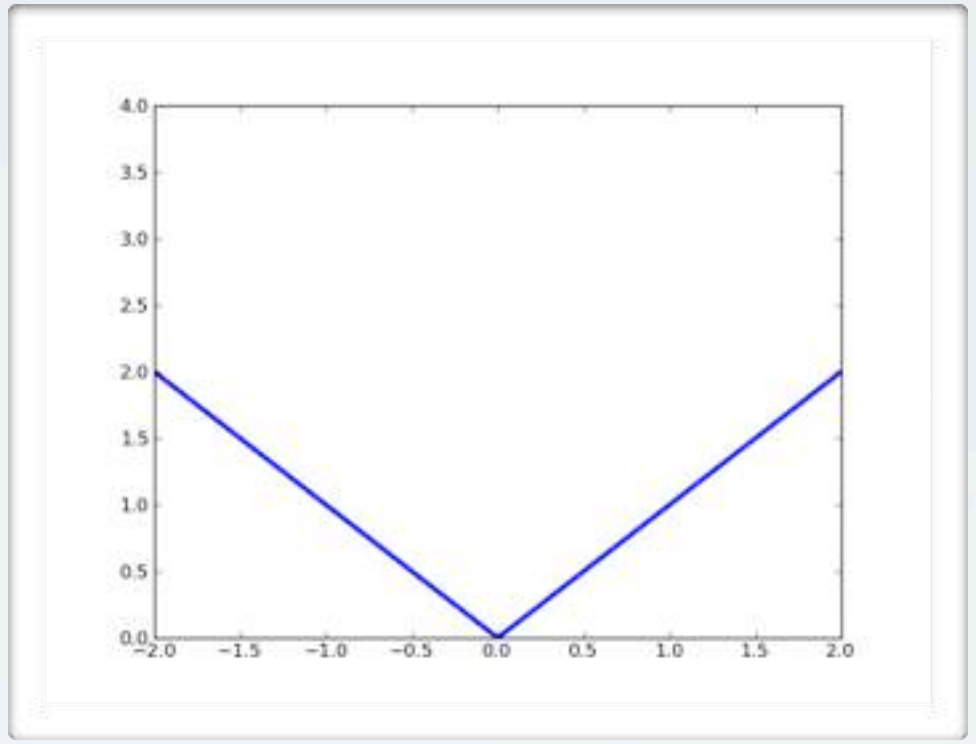
  - $\mathbf{D}$ is equivalent to the autoencoder output weight matrix
  - however, $\mathbf{h}(\mathbf{x}^{(t)})$ is now a complicated function of $\mathbf{x}^{(t)}$
    - encoder is the minimization $\mathbf{h}(\mathbf{x}^{(t)}) = \arg\min_{\mathbf{h}^{(t)}} \frac{1}{2}||\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}^{(t)}||_2^2 + \lambda||\mathbf{h}^{(t)}||_1$

SPARSE CODING

Topics: inference of sparse codes

- Given $\mathbf{D}$, how do we compute $\mathbf{h}(\mathbf{x}^{(t)})$
  - we want to optimize $l(\mathbf{x}^{(t)}) = \frac{1}{2}||\mathbf{x}^{(t)} - \mathbf{D}\,\mathbf{h}^{(t)}||_2^2 + \lambda||\mathbf{h}^{(t)}||_1$ w.r.t. $\mathbf{h}^{(t)}$





  - we could use a gradient descent method:

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

SPARSE CODING

Topics: inference of sparse codes

- For a single hidden unit:

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

  - 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
  - each hidden unit update would be performed as follows:
    - $h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha (\mathbf{D}_{\cdot,k})^\top (\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)})$
    - 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: $h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha\,\lambda\,\mathrm{sign}(h_k^{(t)})$

SPARSE CODING

Topics: inference of sparse codes

- For a single hidden unit:

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

  - 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
  - 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: $h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha\,\lambda\,\mathrm{sign}(h_k^{(t)})$

SPARSE CODING

Topics: inference of sparse codes

- 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
  - each hidden unit update would be performed as follows:

$$\left.\begin{array}{l} \text{- } h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha (\mathbf{D}_{\cdot,k})^\top (\mathbf{D}\ \mathbf{h}^{(t)} - \mathbf{x}^{(t)}) \end{array}\right\} \text{update from reconstruction}$$

$$\left.\begin{array}{l} \text{- if } \operatorname{sign}(h_k^{(t)}) \neq \operatorname{sign}(h_k^{(t)} - \alpha\,\lambda \operatorname{sign}(h_k^{(t)})) \text{ then: } h_k^{(t)} \Longleftarrow 0 \\ \text{- else: } h_k^{(t)} \Longleftarrow h_k^{(t)} - \alpha\,\lambda \operatorname{sign}(h_k^{(t)}) \end{array}\right\} \text{update from sparsity}$$

SPARSE CODING

Topics: ISTA (Iterative Shrinkage and Thresholding Algorithm)

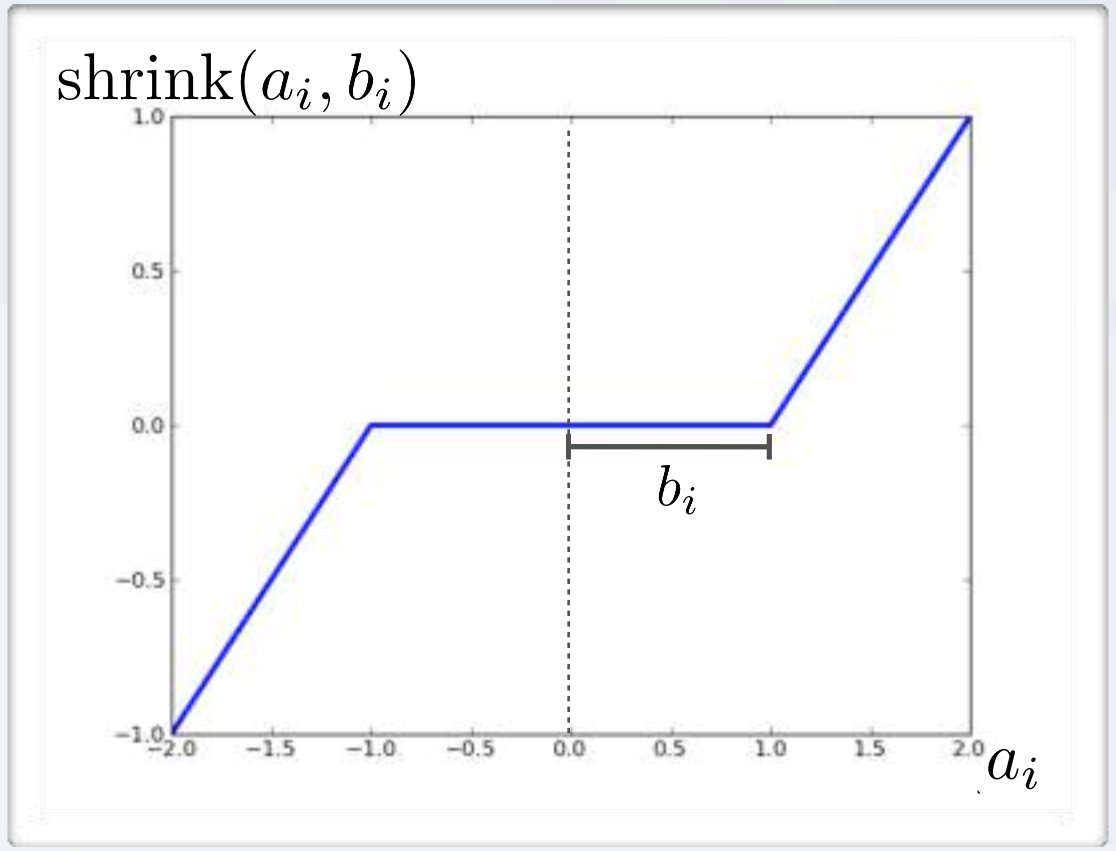
- This process corresponds to the ISTA algorithm:
  - initialize $\mathbf{h}^{(t)}$ (for instance to 0)
  - while $\mathbf{h}^{(t)}$ has not converged
    - $\mathbf{h}^{(t)} \Longleftarrow \mathbf{h}^{(t)} - \alpha\, \mathbf{D}^\top (\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)})$
    - $\mathbf{h}^{(t)} \Longleftarrow \mathrm{shrink}(\mathbf{h}^{(t)}, \alpha\,\lambda)$
  - return $\mathbf{h}^{(t)}$
- Here $\mathrm{shrink}(\mathbf{a}, \mathbf{b}) = [\ldots, \mathrm{sign}(a_i)\ \max(|a_i| - b_i, 0), \ldots]$
- Will converge if $\frac{1}{\alpha}$ is bigger than the largest eigenvalue of $\mathbf{D}^\top\mathbf{D}$

SPARSE CODING

Topics: ISTA (Iterative Shrinkage and Thresholding Algorithm)

- This process corresponds to the ISTA algorithm:

  - initialize $\mathbf{h}^{(t)}$ (for instance to 0)
  - while $\mathbf{h}^{(t)}$ has not converged
    - $\mathbf{h}^{(t)} \Longleftarrow \mathbf{h}^{(t)} - \alpha\, \mathbf{D}^\top(\mathbf{D}\,\mathbf{h}^{(t)} - \mathbf{x}^{(t)})$
    - $\mathbf{h}^{(t)} \Longleftarrow \mathrm{shrink}(\mathbf{h}^{(t)}, \alpha\,\lambda)$
  - return $\mathbf{h}^{(t)}$



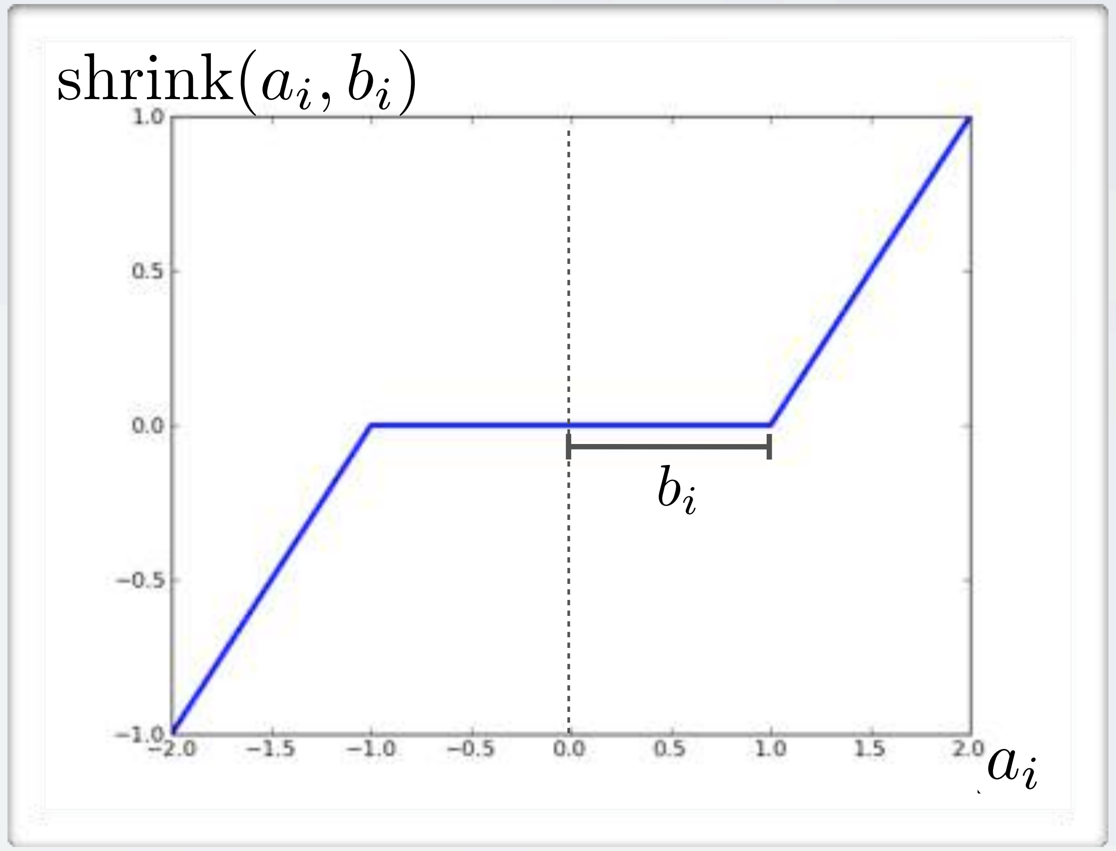
- Here $\mathrm{shrink}(\mathbf{a}, \mathbf{b}) = [\ldots, \mathrm{sign}(a_i)\ \max(|a_i| - b_i, 0), \ldots]$
- Will converge if $\frac{1}{\alpha}$ is bigger than the largest eigenvalue of $\mathbf{D}^\top\mathbf{D}$

SPARSE CODING

Topics: ISTA (Iterative Shrinkage and Thresholding Algorithm)

- This process corresponds to the ISTA algorithm:
  - initialize $\mathbf{h}^{(t)}$ (for instance to 0)
  - while $\mathbf{h}^{(t)}$ has not converged
    - $\mathbf{h}^{(t)} \Longleftarrow \mathbf{h}^{(t)} - \alpha\, \mathbf{D}^\top (\mathbf{D}\, \mathbf{h}^{(t)} - \mathbf{x}^{(t)})$
    - $\mathbf{h}^{(t)} \Longleftarrow \mathrm{shrink}(\mathbf{h}^{(t)}, \alpha\, \lambda)$
  - return $\mathbf{h}^{(t)}$

this is $\mathbf{h}(\mathbf{x}^{(t)})$



- Here $\mathrm{shrink}(\mathbf{a}, \mathbf{b}) = [\ldots, \mathrm{sign}(a_i)\ \max(|a_i| - b_i, 0), \ldots]$
- Will converge if $\frac{1}{\alpha}$ is bigger than the largest eigenvalue of $\mathbf{D}^\top \mathbf{D}$

SPARSE CODING

Topics: coordinate descent for sparse coding inference

- 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

Neural networks

Sparse coding - dictionary update with projected gradient descent

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as much as possible
- More formally:

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} \overbrace{||\mathbf{x}^{(t)} - \underbrace{\mathbf{D}\ \mathbf{h}^{(t)}}_{\text{reconstruction } \widehat{\mathbf{x}}^{(t)}}||_2^2}^{\text{reconstruction error}} + \underbrace{\lambda}_{\text{reconstruction vs. sparsity control}} \overbrace{||\mathbf{h}^{(t)}||_1}^{\text{sparsity penalty}}$$

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

SPARSE CODING

Topics: dictionary update (algorithm 1)

- Going back to our original 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's assume $\mathbf{h}(\mathbf{x}^{(t)})$ doesn't depend on $\mathbf{D}$ (which is false)
  - we must 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 $\mathbf{D}$ to be of unit norm

SPARSE CODING

Topics: dictionary update (algorithm 1)

- A gradient descent method could be used here too
  - specifically, this is a projected gradient descent algorithm

- While $\mathbf{D}$ hasn't converged
  - perform gradient update of $\mathbf{D}$

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

  - renormalize the columns of $\mathbf{D}$
    - for each column $\mathbf{D}_{\cdot,j}$:

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

Neural networks

Sparse coding - dictionary update with block-coordinate descent

SPARSE CODING

Topics: dictionary update (algorithm 2)

- Going back to our original 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's assume $\mathbf{h}(\mathbf{x}^{(t)})$ doesn't depend on $\mathbf{D}$ (which is false)
  - we must 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 $\mathbf{D}$ to be of unit norm

SPARSE CODING

Topics: dictionary update (algorithm 2)

- An alternative is to solve for each column $\mathbf{D}_{\cdot,j}$ in cycle:
  - setting the gradient for $\mathbf{D}_{\cdot,j}$ to zero, we have

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

  - we <u>don't need to specify a learning rate</u> to update $\mathbf{D}_{\cdot,j}$

SPARSE CODING

Topics: dictionary update (algorithm 2)

- An alternative is to solve for each column $\mathbf{D}_{\cdot,j}$ in cycle:
  - we can rewrite

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

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

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

  - this way, we only need to store:
    - $\mathbf{A} \Longleftarrow \sum_{t=1}^{T} \mathbf{h}(\mathbf{x}^{(t)})\ \mathbf{h}(\mathbf{x}^{(t)})^\top$
    - $\mathbf{B} \Longleftarrow \sum_{t=1}^{T} \mathbf{x}^{(t)}\ \mathbf{h}(\mathbf{x}^{(t)})^\top$

SPARSE CODING

Topics: dictionary update (algorithm 2)

- While $\mathbf{D}$ hasn't converged
  - for each column $\mathbf{D}_{\cdot,j}$ perform updates
    - $\mathbf{D}_{\cdot,j} \Longleftarrow \dfrac{1}{A_{j,j}} \left(\mathbf{B}_{\cdot,j} - \mathbf{D}\ \mathbf{A}_{\cdot,j} + \mathbf{D}_{\cdot,j}\ A_{j,j}\right)$
    - $\mathbf{D}_{\cdot,j} \Longleftarrow \dfrac{\mathbf{D}_{\cdot,j}}{||\mathbf{D}_{\cdot,j}||_2}$

- 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 $\mathbf{D}_{\cdot,j}$

Neural networks

Sparse coding - dictionary learning algorithm

SPARSE CODING

Topics: 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 $\mathbf{x}^{(t)}$ as much as possible
- More formally:

$$\min_{\mathbf{D}} \frac{1}{T} \sum_{t=1}^{T} \min_{\mathbf{h}^{(t)}} \frac{1}{2} \overbrace{||\mathbf{x}^{(t)} - \underbrace{\mathbf{D}\,\mathbf{h}^{(t)}}_{\text{reconstruction } \widehat{\mathbf{x}}^{(t)}}||_2^2}^{\text{reconstruction error}} + \underbrace{\lambda}_{\text{reconstruction vs. sparsity control}} \overbrace{||\mathbf{h}^{(t)}||_1}^{\text{sparsity penalty}}$$

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

SPARSE CODING

Topics: learning algorithm (putting it all together)

- Learning alternates between inference and dictionary learning

- While $\mathbf{D}$ has not converged
  - find the sparse codes $\mathbf{h}(\mathbf{x}^{(t)})$ for all $\mathbf{x}^{(t)}$ in my 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 $\mathbf{D}$

- Similar to the EM algorithm

Neural networks

Sparse coding - online dictionary learning algorithm

SPARSE CODING

Topics: learning algorithm (putting it all together)

- Learning alternates between inference and dictionary learning

- While $\mathbf{D}$ has not converged
  - find the sparse codes $\mathbf{h}(\mathbf{x}^{(t)})$ for all $\mathbf{x}^{(t)}$ in my 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 $\mathbf{D}$

- Similar to the EM algorithm

SPARSE CODING

Topics: online learning algorithm

- This algorithm is "batch" (i.e. not online)
  - single update of the dictionary per pass on the training set
  - for large datasets, we'd like to update $\mathbf{D}$ after visiting each $\mathbf{x}^{(t)}$
- Solution: for each $\mathbf{x}^{(t)}$
  - perform inference of $\mathbf{h}(\mathbf{x}^{(t)})$ for the current $\mathbf{x}^{(t)}$
  - update running averages of the quantities required to update $\mathbf{D}$:
    - $\mathbf{B} \Longleftarrow \beta\,\mathbf{B} + (1-\beta)\,\mathbf{x}^{(t)}\,\mathbf{h}(\mathbf{x}^{(t)})^\top$
    - $\mathbf{A} \Longleftarrow \beta\,\mathbf{A} + (1-\beta)\,\mathbf{h}(\mathbf{x}^{(t)})\,\mathbf{h}(\mathbf{x}^{(t)})^\top$
  - use current value of $\mathbf{D}$ as "warm start" to block-coordinate descent

SPARSE CODING

Topics: online learning algorithm

- Initialize $\mathbf{D}$ (not to 0!)
- While $\mathbf{D}$ hasn't converged
  - for each $\mathbf{x}^{(t)}$
    - infer code $\mathbf{h}(\mathbf{x}^{(t)})$
    - update dictionary
      - ✓ $\mathbf{B} \Longleftarrow \beta\, \mathbf{B} + (1-\beta)\, \mathbf{x}^{(t)}\, \mathbf{h}(\mathbf{x}^{(t)})^\top$
      - ✓ $\mathbf{A} \Longleftarrow \beta\, \mathbf{A} + (1-\beta)\, \mathbf{h}(\mathbf{x}^{(T+1)})\, \mathbf{h}(\mathbf{x}^{(T+1)})^\top$
      - ✓ while $\mathbf{D}$ hasn't converged
        - ★ for each column $\mathbf{D}_{\cdot,j}$ perform gradient update

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

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

Online Dictionary Learning for Sparse Coding. Mairal, Bach, Ponce and Sapiro, 2009.

Neural networks

Sparse coding - ZCA preprocessing

PREPROCESSING

Topics: ZCA

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

PREPROCESSING

Topics: ZCA

- After this transformation
  - the empirical mean is 0

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

PREPROCESSING

Topics: ZCA

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

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

Neural networks

Sparse coding - feature extraction

FEATURE EXTRACTION

Topics: feature learning

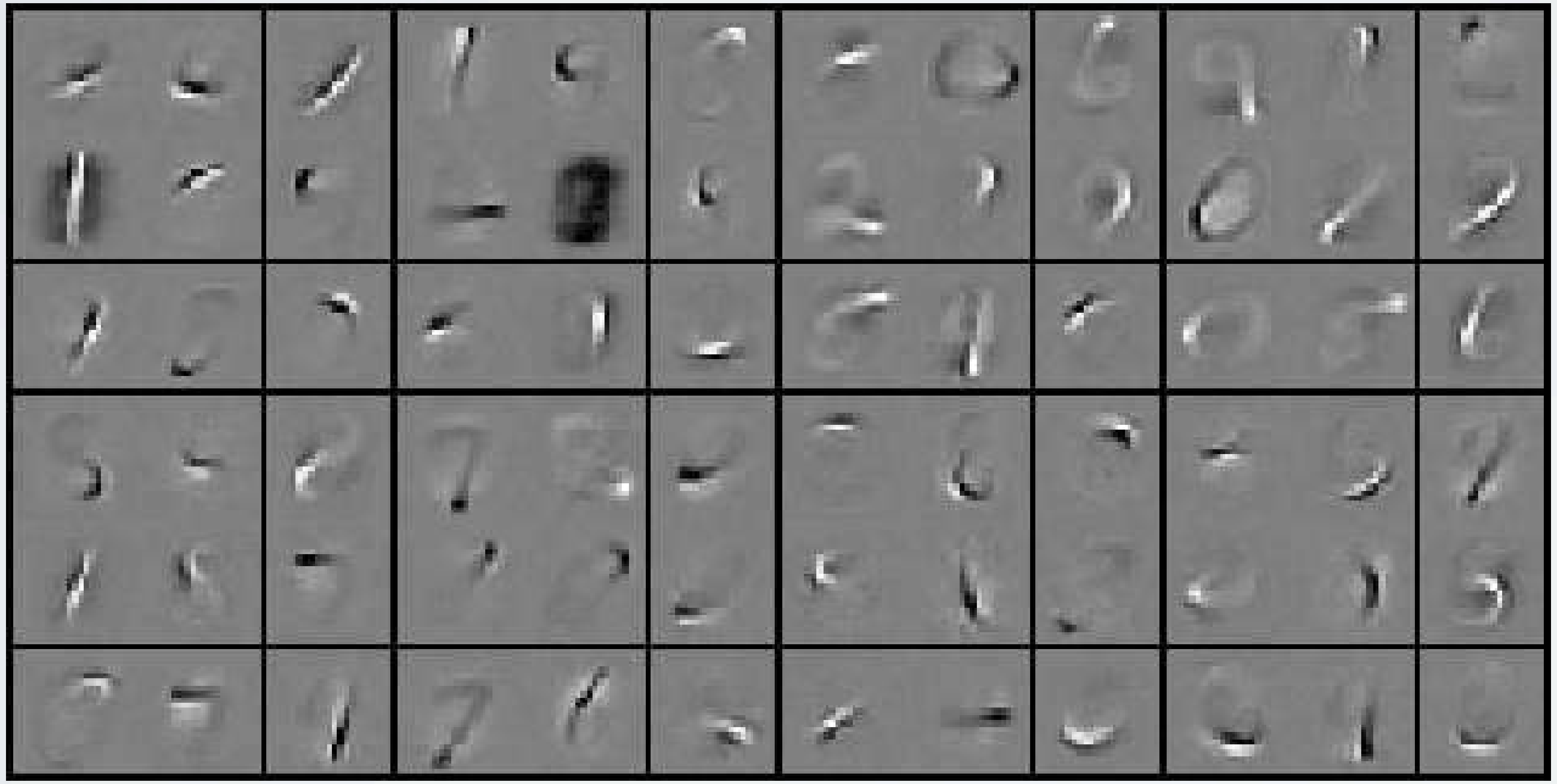
- A sparse coding model can be used to extract features
  - given a labeled training set $\{(\mathbf{x}^{(t)}, y^{(t)})\}$
  - train sparse coding dictionary only on training inputs $\{\mathbf{x}^{(t)}\}$
    - this yields a dictionary $\mathbf{D}$ from which to infer sparse codes $\mathbf{h}(\mathbf{x}^{(t)})$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

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

FEATURE EXTRACTION

Topics: feature learning

- When trained on handwritten digits:



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

FEATURE EXTRACTION

Topics: 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 Data
Raina, Battle, Lee, Packer and Ng.

Neural networks

Sparse coding - relationship with V1

RELATIONSHIP WITH V1

Topics: V1 neurons vs. sparse coding

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

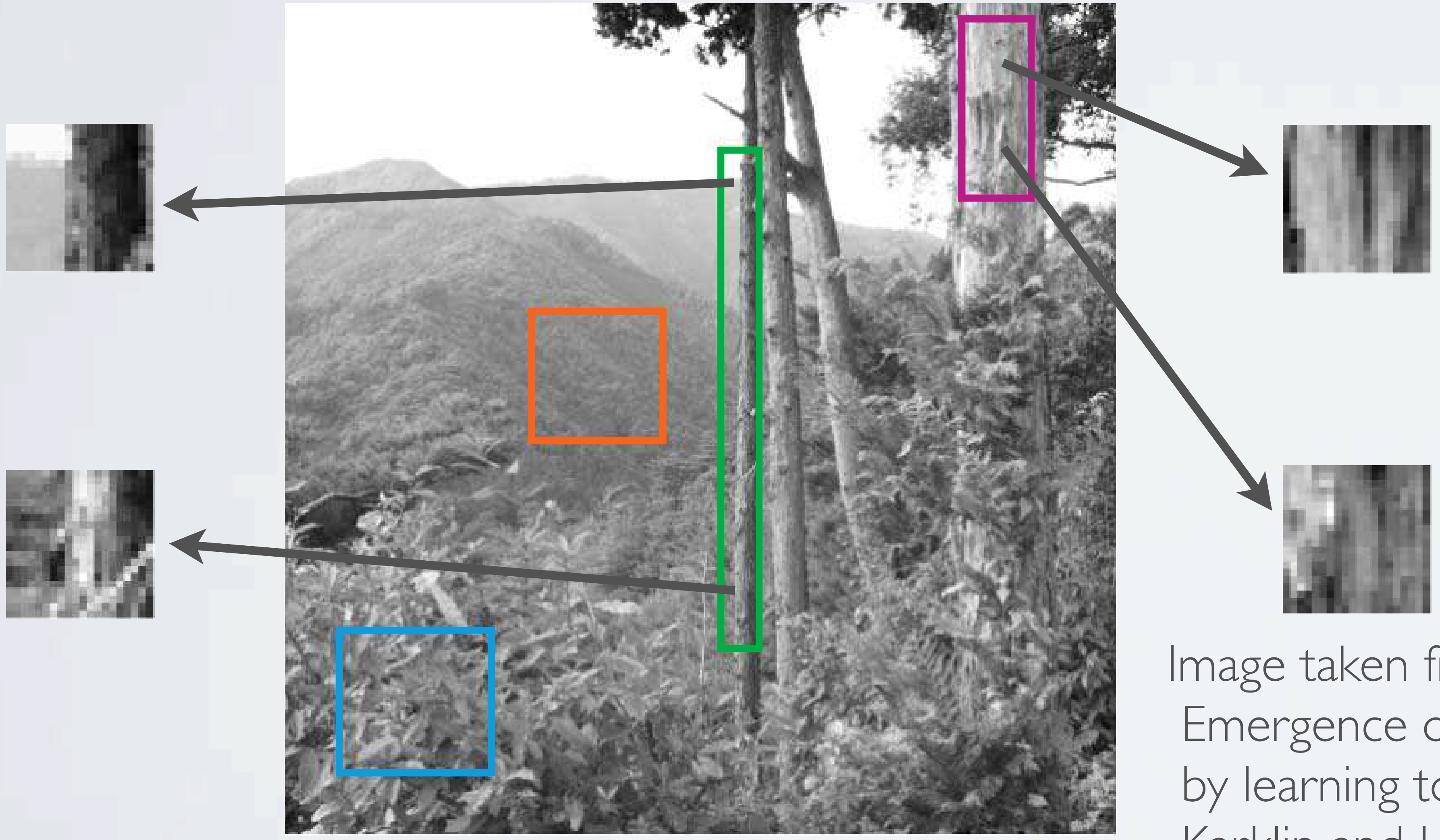
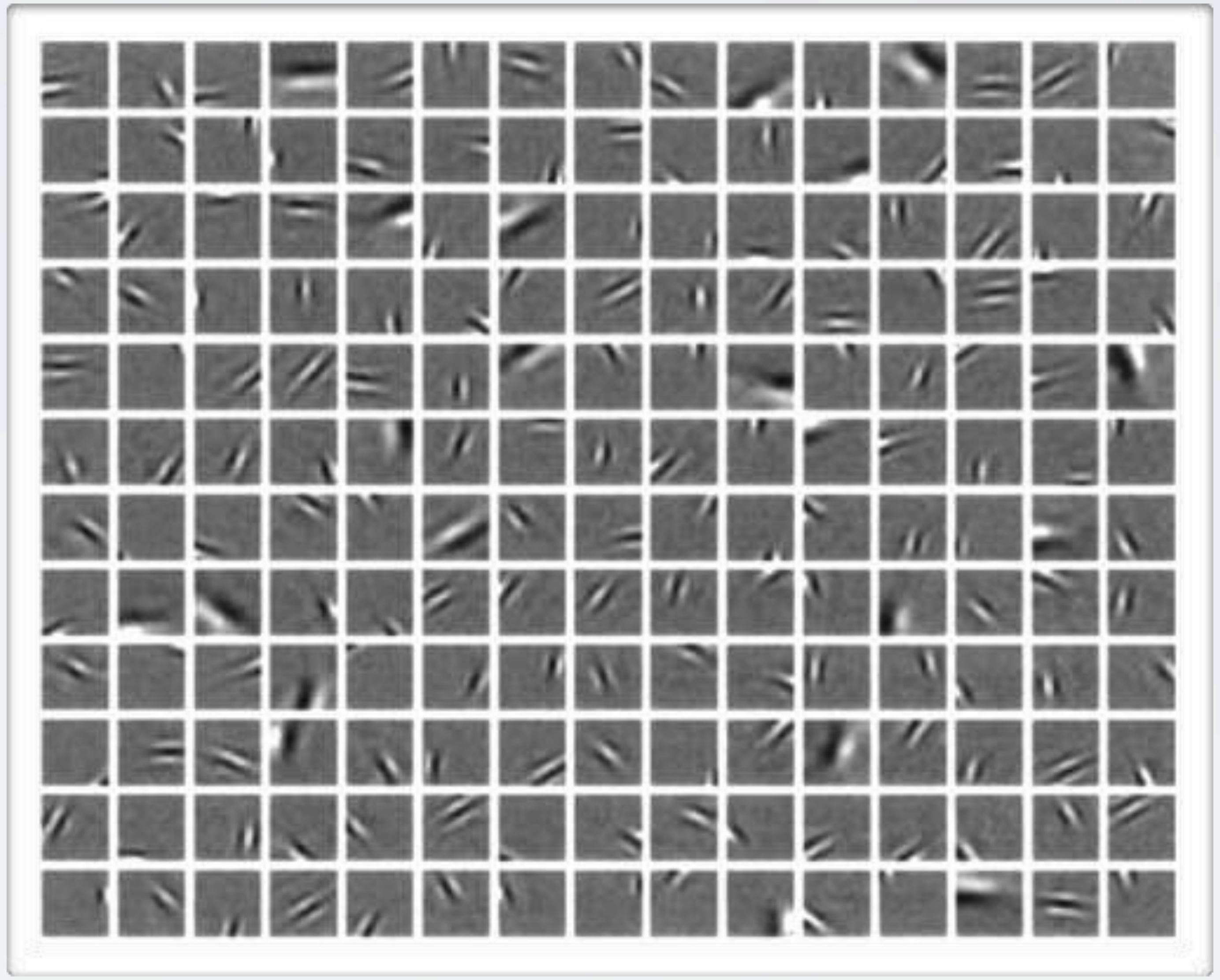


Image taken from:
Emergence of complex cell properties
by learning to generalize in natural scenes.
Karklin and Lewicki, 2009

RELATIONSHIP WITH V1

Topics: V1 neurons vs. sparse coding

- 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



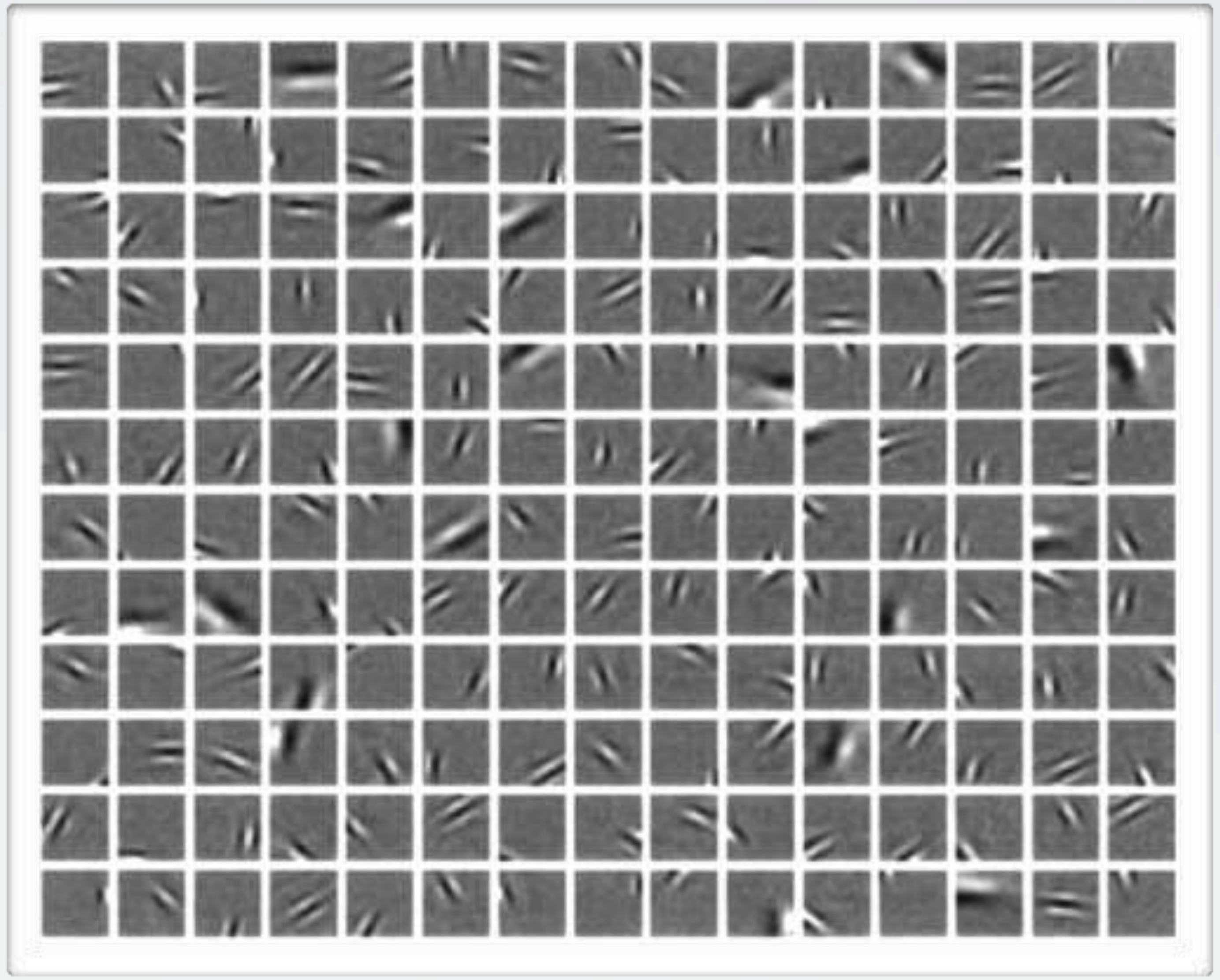
Emergence of simple-cell receptive field properties by learning a sparse code of natural images. Olshausen and Field, 1996.

RELATIONSHIP WITH V1

Topics: V1 neurons vs. sparse coding

- 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.