Autoencoders, Extensions, and Applications

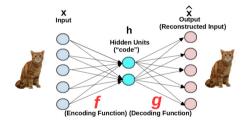
Piyush Rai

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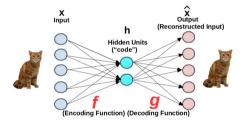
- Introduction to Autoencoders
- Autoencoder Variants and Extensions
- Some Applications of Autoencoders
- Autoencoders for Recommender Systems

- Similar to the standard feedforward neural network with a key difference:
 - Unsupervised. No "label" at the output layer; Output layer simply tries to "recreate" the input



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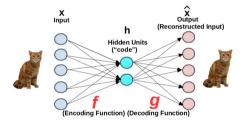
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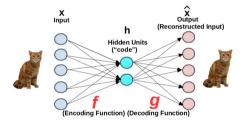
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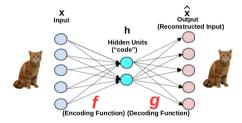
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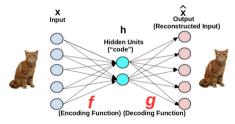
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- For an Autoencoder, f and g are learned with a goal to minimize the difference between \hat{x} and x

Autoencoder for Feature Learning

• The learned code h = f(x) can be used as a new feature representation of the input x

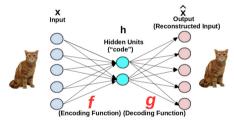


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Autoencoder for Feature Learning

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- Note: Size of the hidden units (encoding) can also be larger than the input

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- Let's assume a $D \times 1$ input $\pmb{x} \in \mathbb{R}^D$, and a single hidden layer with $K \times 1$ code $\pmb{h} \in \mathbb{R}^K$
- We can then define a simple linear autoencoder as

$$h = f(x) = Wx + b$$

$$\hat{x} = g(h) = W^*h + c$$

where f is defined by $\mathbf{W} \in \mathbb{R}^{K \times D}$ and $\mathbf{b} \in \mathbb{R}^{K \times 1}$

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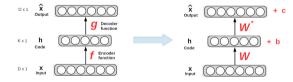
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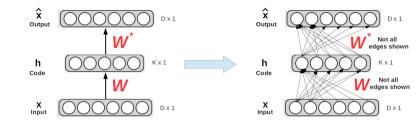
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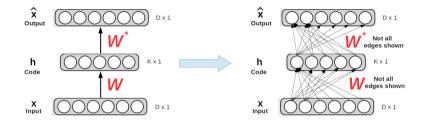


• Note: If we learn f, g to minimize the squared error $||\hat{x} - x||^2$ then the linear autoencoder with $\mathbf{W}^* = \mathbf{W}^\top$ is optimal, and is equivalent to Principal Component Analysis (PCA)

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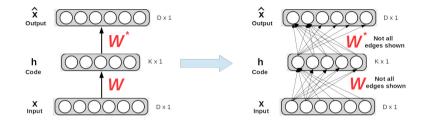
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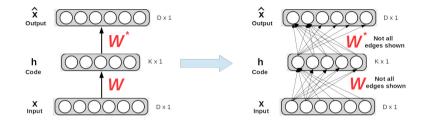
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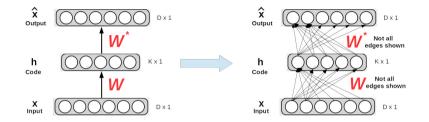
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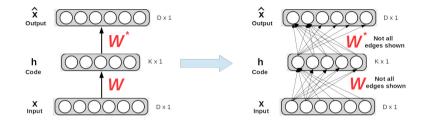
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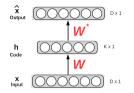


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- If $\mathbf{W}^* = \mathbf{W}^{\top}$, the autoencoder architecture is said to have "tied weights"

Nonlinear Autoencoders

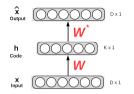


- The hidden nodes can also be nonlinear transforms of the inputs, e.g.,
 - Can define h as a linear transform of x followed by a nonlinearity (e.g., sigmoid, ReLU)

$$h = sigmoid(Wx + b)$$

where the nonlinearity sigmoid(z) = $\frac{1}{1+\exp(-z)}$ squashes the real-valued z to lie between 0 and 1

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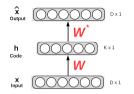
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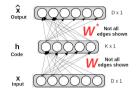
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- Most commonly used autoencoders use such nonlinear transforms
- Note: If inputs $\mathbf{x} \in \{0,1\}^D$ are binary, it may be more appropriate to also define $\hat{\mathbf{x}}$ as

 $\hat{\boldsymbol{x}} = \operatorname{sigmoid}(\boldsymbol{W}^* \boldsymbol{h} + \boldsymbol{c})$

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What's Learned by an Autoencoder?

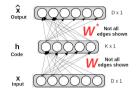


• Figure below: The $K \times D$ matrix **W** learned on digits data. Each tiny block visualizes a row of **W**

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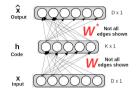
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- Thus W captures the possible "patterns" in the training data (akin to the K basis vectors in PCA)
- For any input x, the encoding h tells us how much each of these K features in present in x

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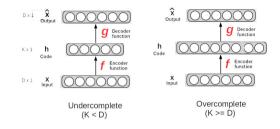
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- We find (W, b, W*, c) by minimizing the reconstruction error (summed over all training data)
- This can be done using backpropagation

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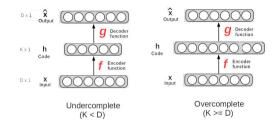
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Undercomplete, Overcomplete, and Need for Regularization



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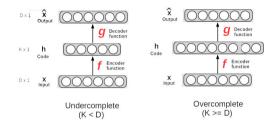


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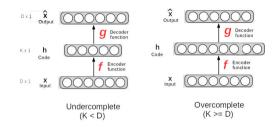
Undercomplete, Overcomplete, and Need for Regularization



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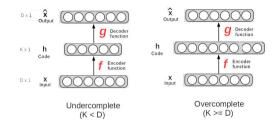
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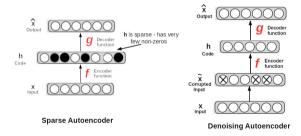


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- Overcomplete: Imagine K ≥ D and trivial (identity) functions f and g. Can achieve even zero reconstruction error but the learned code will not capture any interesting properties in the data
- It is therefore important to regularize the functions as well as the learned code, and not just focus on minimizing the reconstruction error

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Regularized Autoencoders

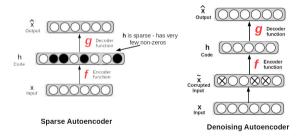
- Several ways to regularize the model, e.g.
 - Make the learned code sparse (Sparse Autoencoders)
 - Make the model robust against noisy/incomplete inputs (Denoising Dutoencoders)



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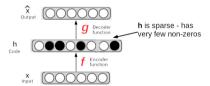
• Make the model robust against small changes in the input (Contractive Autoencoders)

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• Make the learned code sparse (Sparse Autoencoders). Done by adding a sparsity penalty on \boldsymbol{h}

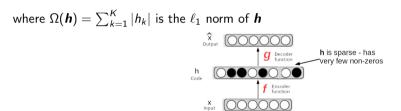
Loss Function: $\ell(\hat{\boldsymbol{x}}, \boldsymbol{x}) + \Omega(\boldsymbol{h})$

where $\Omega(\boldsymbol{h}) = \sum_{k=1}^{K} |h_k|$ is the ℓ_1 norm of \boldsymbol{h}



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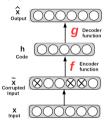
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• Sparse autoencoder is learned by minimizing the above regularized loss function

Denoising Autoencoders

- First add some noise (e.g., Gaussian noise) to the original input x
- Let's denote \tilde{x} as the corrupted version of x
- The encoder f operates on \tilde{x} , i.e., $h = f(\tilde{x})$



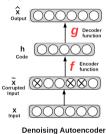
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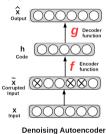
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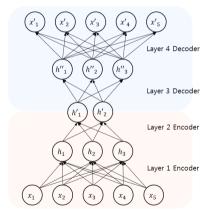


- However, we still want to reconstruction \hat{x} to be close to the original uncorrupted input x
- Since the corruption is stochastic, we minimize the expected loss: $\mathbb{E}_{\tilde{\mathbf{x}} \sim p(\tilde{\mathbf{x}}|\mathbf{x})}[\ell(\hat{\mathbf{x}}, \tilde{\mathbf{x}})] + \Omega(\mathbf{h})$

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Deep/Stacked Autoencoders

• Most autoencoders can be extended to have more than one hidden layer



• Can also define the encoder and decoder functions using probability distributions

 $p_{ ext{encoder}}(m{h}|m{x}) \ p_{ ext{decoder}}(m{x}|m{h})$

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- Negative log-likelihood $-\log p_{decoder}(\boldsymbol{x}|\boldsymbol{h})$ is equivalent to the reconstruction error

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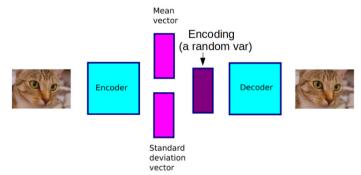
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- Such ideas have been used to design generative models for autoencoders
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 - ullet Generative models like VAE can be used to "generate" new data using a random code $m{h}$

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Variational Autoencoders (VAE)

• Learns a distribution (e.g., a Gaussian) on the encoding¹



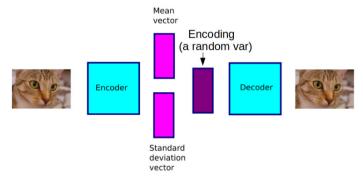
¹http://www.birving.com/presentations/autoencoders/

Piyush Rai (IIT Kanpur)

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Variational Autoencoders (VAE)

• Learns a distribution (e.g., a Gaussian) on the encoding¹



• Unlike standard AE, a VAE model learns to generate plausible data from random encodings

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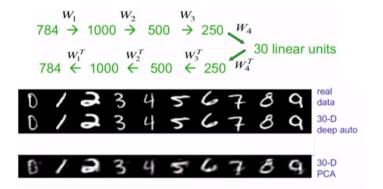
- (Unsupervised) Feature learning and Dimensionality reduction
- Denoising and inpainting
- Pre-training of deep neural networks
- Recommender systems applications

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Feature learning and Dimensionality Reduction

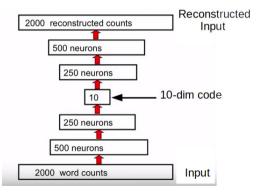
• Example: A deep AE for low-dim feature learning for 784-dimensional MNIST images²



²Figure credit: Hinton and Salakhutdinov

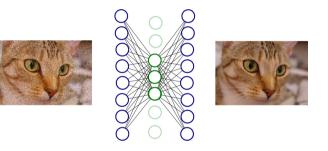
Feature learning and Dimensionality Reduction

• Example: Low-dim feature learning for 2000-dimensional bag-of-words documents

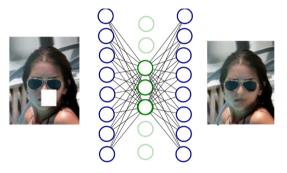


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Denoising and Inpainting



Denoising and Inpainting



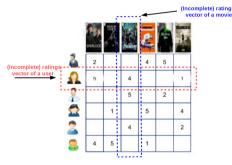
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Applications in Recommender Systems

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Recommender Systems

• Assume we are given a partially known $N \times M$ ratings matrix **R** of N users on M items (movies)

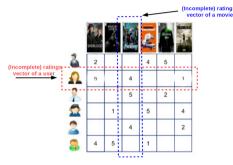


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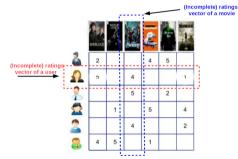


- Denote by $\mathbf{r}^{(u)}$ the (partially known) $M \times 1$ ratings vector of user u
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- How can we use this data to build a recommender system?

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Recommender Systems via Matrix Completion

• An idea: If the predicted value of a user's rating for a movie is high, then we should ideally recommend this movie to the user

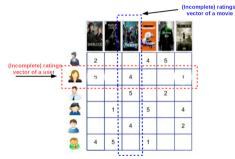


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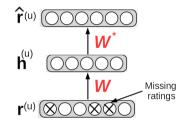


• Thus if we can "reconstruct" the missing entries in **R**, we can use this method to recommend movies to users. Using an autoencoders can help us do this!

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An Autoencoder based Approach

• Using the rating vectors $\{\mathbf{r}^{(u)}\}_{u=1}^N$ of all users, can learn an autoencoder



 \bullet Note: During backprop, only update weights in ${\bf W}$ that are connected to the observed ratings^3

• Once learned, the model can predict (reconstruct) the missing ratings

Another Autoencoder based Approach

• Another approach is to combine (denoising) autoencoders with a matrix factorization model⁴

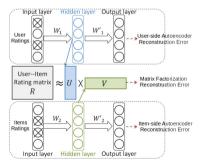
⁴Deep Collaborative Filtering via Marginalized Denoising Auto-encoder (Li et al, CIKM:2015) アト・モントモント ミークへへ

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- Idea: Rating of a user u on an item i can be defined using the inner-product based similarity of their features learned via an autoencoder: $R_{ui} = f(\mathbf{h}^{(u)^{\top}} \mathbf{h}^{(i)})$ where f is some compatibity function

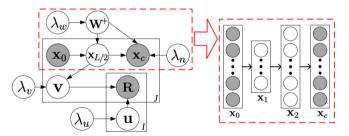
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- Denoting $\{\boldsymbol{h}^{(u)}\}_{u=1}^{N} = \boldsymbol{\mathsf{U}}$ and $\{\boldsymbol{h}^{(i)}\}_{i=1}^{M} = \boldsymbol{\mathsf{V}}$, we can write $\boldsymbol{\mathsf{R}} = \boldsymbol{\mathsf{U}}\boldsymbol{\mathsf{V}}^{\top}$



Other Approaches on Autoencoders for Recommender Systems

- Several recent papers on similar autoencoder based ideas
 - Collaborative Denoising Auto-Encoders for Top-N Recommender Systems (Wu et al, WSDM 2016)
 - Collaborative Deep Learning for Recommender Systems (Wang et al, KDD 2015)



• Also possible to incorporate side information about the users and/or items (Wang et al, KDD 2015)

- Simple and powerful for (nonlinear) feature learning
- Learned features are able to capture salient properties of data
- Several extensions (sparse, denoising, stochastic, etc.)
- Can also be stacked to create "deep" autoencoders
- Recent focus on autoencoders that are based on generative models of data
 - Example: Variational Autoencoders