Deep Learning II : unsupervised tasks with Auto-encoders
Data Science Bootcamp

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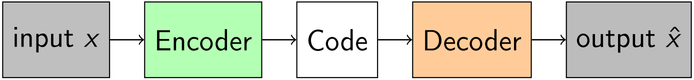
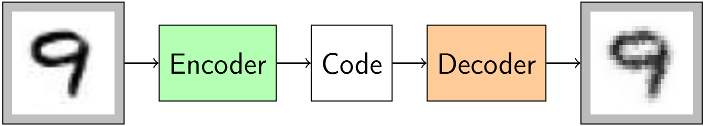
Agenda

General architecture of a Deep Autoencoder



General architecture of a Deep Autoencoder



Autoencoders basics: encoder and decoder

Encoder

Produces Code or Latent Representation

$$\mathbf{h} = s(\mathbf{W}\mathbf{x} + \mathbf{b}) = f(\mathbf{x})$$

Decoder

Produces Reconstruction of the input

$$\hat{\mathbf{x}} = s(\mathbf{W}'\mathbf{h} + \mathbf{b}') = g(\mathbf{h})$$

Tied weights when $\mathbf{W}' = \mathbf{W}^T$

Autoencoders basics: loss function

Given the output $\hat{\mathsf{x}} = g(f(\mathsf{x}))$
We want to minimize some reconstruction loss:

$$\mathcal{L}(\mathsf{x}, g(f(\mathsf{x})) = \hat{\mathsf{x}})$$

Cross entropy (bits or probability vectors)

$$\mathcal{L}(\mathsf{x}, \hat{\mathsf{x}}) = \mathsf{x} \log \hat{\mathsf{x}} + (1 - \mathsf{x}) \log(1 - \hat{\mathsf{x}})$$

Mean squared error (continuous values)

$$\mathcal{L}(\mathsf{x}, \hat{\mathsf{x}}) = ||\mathsf{x} - \hat{\mathsf{x}}||^2$$

Autoencoders basics: flavours

Undercomplete

- Bottleneck layer produces code $\mathbf{h}$ with less dimensions then input $\mathbf{x}$

Overcomplete

- Code $\mathbf{h}$ has more dimensions then the input $\mathbf{x}$
- Different versions e.g. sparse, denoising, contractive.

Agenda

Autoencoders basics

Undercomplete AEs

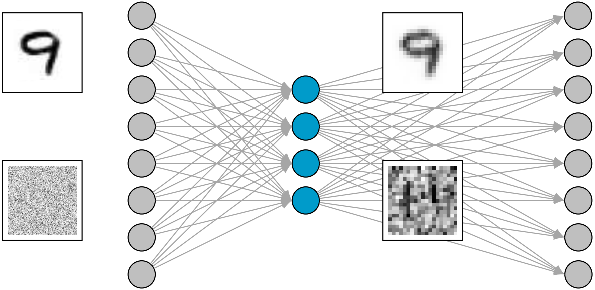
Overcomplete Regularized AEs

Concluding remarks

Undercomplete

Learns a Lossy Compression of the input data.

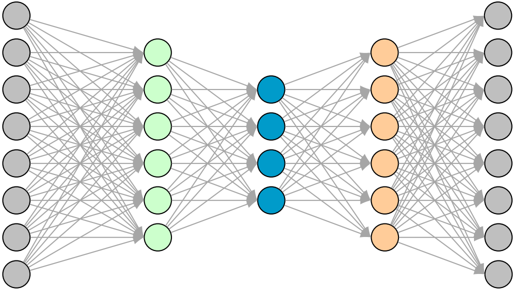
- has a “bottleneck” layer
- can be used for Dimensionality Reduction — often compared to Principal Component Analysis (PCA)
- often code is a good representation for the training data only



Undercomplete

Increasing the number of layers adds capacity to the AE.

- Encoder and Decoder layers can also be convolutional layers



In principle with a sufficiently large capacity it may map every input to a single neuron on bottleneck layer.

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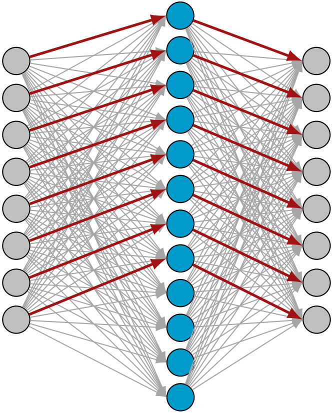
Overcomplete AEs

High-dimensional intermediate layer

- a naive implementation would allow a copy so that $\mathbf{x} = \hat{\mathbf{x}}$



Overcomplete regularized AEs

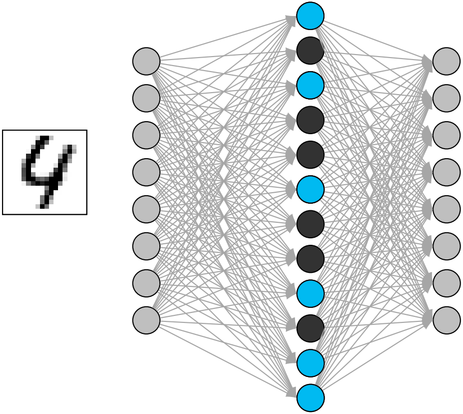
Regularization with sparsity constraint

$$\mathcal{L}(x, g(f(x))) + \Omega(f(x))$$
$$\mathcal{L}(x, g(f(x))) + \lambda \sum_i |h_i|,$$

- loss function tries to keep a low number of activation neurons per training input

Overcomplete regularized AEs

Regularization with sparsity constraint



Denoising AEs (DAEs)

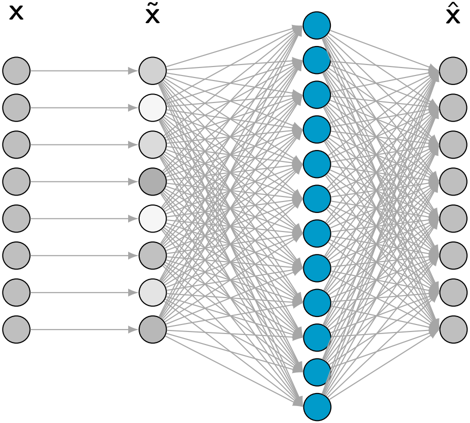
Regularization achieved by adding noise to $\mathbf{x}$

- the loss is computed using the noiseless input $\mathbf{x}$
- AE has to reconstruct $\mathbf{x}$ using a noisy input $\tilde{\mathbf{x}}$, so representation must be robust to noise
- this prevents the overcomplete AE to simply copy the data

Denoising AEs (DAEs)

Regularization achieved by adding noise to $\mathbf{x}$

- DAEs aim to learn a good internal representation as a side effect of learning to denoise the input



Denoising AEs (DAEs)

Noise processes

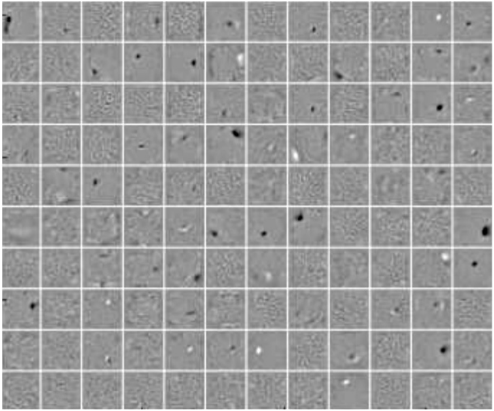
- Additive Gaussian Noise with $\mu = 0$, and some σ;
- Set a percentage of the input data to zero with some probability p.

Interpretation

- Learns to project data around some manifold to the distribution of the original (noiseless) data
- If some input is to far from the original distribution, it produces a high reconstruction error

Denoising AEs (DAEs): example

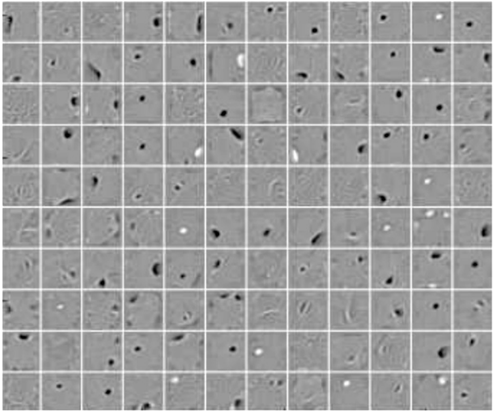
Using MNIST dataset, without noise



Vincent, Pascal, et al. "Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion." Journal of Machine Learning Research, 2010: 3371-3408.

Denoising AEs (DAEs): example

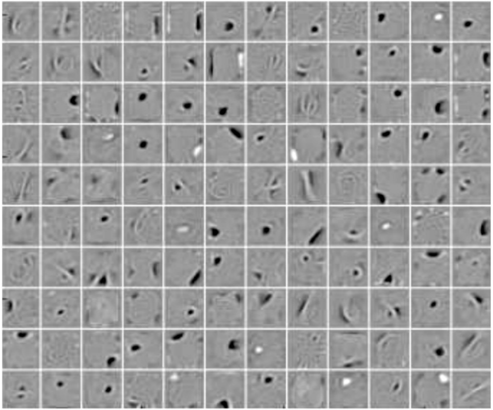
Using MNIST dataset, zero input variable with 25% probability



Vincent, Pascal, et al. "Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion." Journal of Machine Learning Research, 2010: 3371-3408.

Denoising AEs (DAEs): example

Using MNIST dataset, zero input variable with 50% probability



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Contractive AEs (CAEs)

Regularization based on the gradient of code $f(\mathbf{x}) = \mathbf{h}$ with respect to $\mathbf{x}$

- adds a term to the Loss function
- it is referred to as the Frobenius norm of the Jacobian of the Encoder

$$\ell(\mathbf{x}_i, g(f(\mathbf{x}_i))) + \lambda ||\nabla_{\mathbf{x}_i} f(\mathbf{x}_i)||_F^2$$

$$\ell(\mathbf{x}_i, g(f(\mathbf{x}_i))) + \lambda \sum_j \sum_k \left(\frac{\partial f(\mathbf{x}_i)_j}{\partial x_i^{(k)}} \right)^2$$

j – index for the code (intermediate layer unit)
k – index for the input vector

The Jacobian is a matrix of the derivatives of all elements of the code with respect to all elements of the input

Contractive AEs (CAEs)

Effects of terms on the encoder:

- $\ell(\mathbf{x}_i, g(f(\mathbf{x}_i)))$: relies on keeping relevant information;
- $\lambda||\nabla_{\mathbf{x}_i} f(\mathbf{x}_i)||_F^2$: throws away changes in code with respect to input.

Interpretations:

- rate of change of the code must follow the rate of change of the input;
- if noise is added to input, the code should not be affected (compare to Denoising AEs!);
- a good balance between terms will result in keeping only the relevant information.

Contractive AEs (CAEs)

Jacobian matrix can be seen as a linear approximation of a nonlinear encoder.

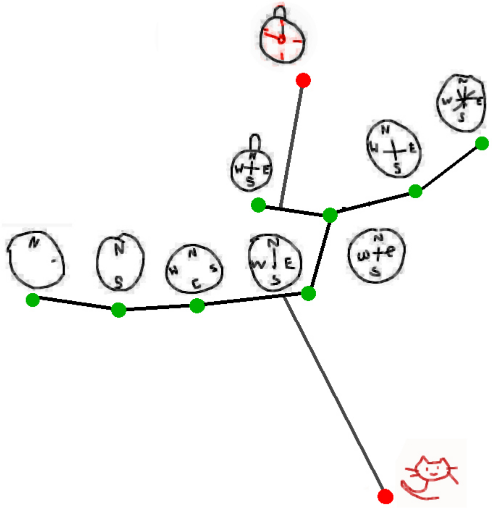
- A linear operator is said to be contractive if the norm of $\mathbf{J_x}$ is kept less than or equal to 1 for all unit-norm of x, i.e. if it shrinks the unit sphere around each point;
- CAE encourages each of the local linear operators to become a contraction;
- only a few directions of the manifold of the data approaches zero, likely the directions approximating the tangent planes of the manifold.

Contractive AEs (CAEs): interpretation for images

CAE learns to reconstruct data that is:

- tangent to the manifold or within some sphere;
- those are likely to represent real variations of the data
- in images that would be related to rotation, style change, etc.

Contractive AEs (CAEs): a sketch manifold illustration



Concluding remarks

- AEs can be a good choice with unsupervised data;
- Deep autoencoders can be useful to many applications, via manifold learning;
- The potential for manifold learning can be used for instance on Generative tasks (Generative and Variational Autoencoders).
- Those can also be plugged in supervised architectures.

References

- **Ponti, M.; Paranhos da Costa, G. Como funciona o Deep Learning. Tópicos em Gerenciamento de Dados e Informações. 2017.**
- **Ponti, M.; Ribeiro, L.; Nazare, T.; Bui, T.; Collomosse, J. Everything you wanted to know about Deep Learning for Computer Vision but were afraid to ask. In: SIBGRAPI – Conference on Graphics, Patterns and Images, 2017.** `http://sibgrapi.sid.inpe.br/rep/sid.inpe.br/sibgrapi/2017/09.05.22.09`
- Rifai, Salah, et al. "Higher order contractive auto-encoder." Machine Learning and Knowledge Discovery in Databases (2011): 645-660.
- Vincent, Pascal, et al. "Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion." Journal of Machine Learning Research, 2010: 3371-3408.
- Goodfellow, Ian, Yoshua Bengio, and Aaron Courville. Deep learning. MIT press, 2016.