Introduction to Statistical Machine Learning

Cheng Soon Ong & Christian Walder

Machine Learning Research Group
Data61 | CSIRO
and
College of Engineering and Computer Science
The Australian National University

Canberra
February – June 2019

(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Part VI

Neural Network 3

Number of layers

- expression of a function is compact when it has few computational elements, i.e. few degrees of freedom that need to be tuned by learning
- for a fixed number of training examples, expect that compact representations of the target function would yield better generalization
- Example representations
  - affine operations, sigmoid $\Rightarrow$ logistic regression has depth 1, fixed number of units (a.k.a. neurons)
  - fixed kernel, affine operations $\Rightarrow$ kernel machine (e.g. SVM) has two levels, with as many units as data points
  - stacked neural network of multiple "linear transformation followed by a non-linearity" $\Rightarrow$ deep neural network has arbitrary depth with arbitrary number of units per layer

Easier to represent with more layers

An old result:

- functions that can be compactly represented by a depth k architecture might require an exponential number of computational elements to be represented by a depth $k-1$ architecture
- Example, the d bit parity function

$$\text{parity} : (b_1, \dots, b_d) \in \{0,1\}^d \mapsto \begin{cases} 1 & \text{if} \quad \sum_{i=1}^{d} b_i \quad \text{is even} \\ 0 & \text{otherwise} \end{cases}$$

- Theorem: d-bit parity circuits of depth 2 have exponential size

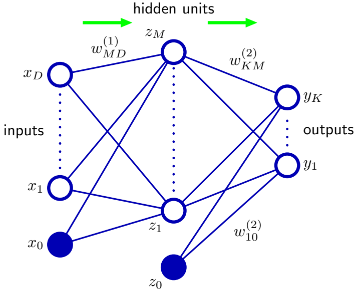
Analogous in modern deep learning:

- “Shallow networks require exponentially more parameters for the same number of modes” — Canadian deep learning mafia.

Recall: Multi-layer Neural Network Architecture

$$y_k(\mathbf{x}, \mathbf{w}) = g\left(\sum_{j=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)$$

where $\mathbf{w}$ now contains all weight and bias parameters.

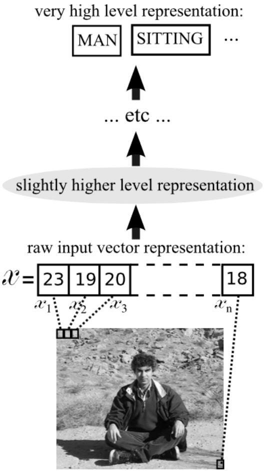


We could add more hidden layers

Empirical observations - pre 2006

- Deep architectures get stuck in local minima or plateaus
- As architecture gets deeper, more difficult to obtain good generalisation
- Hard to initialise random weights well
- 1 or 2 hidden layers seem to perform better
- 2006: Unsupervised pre-training, find distributed representation

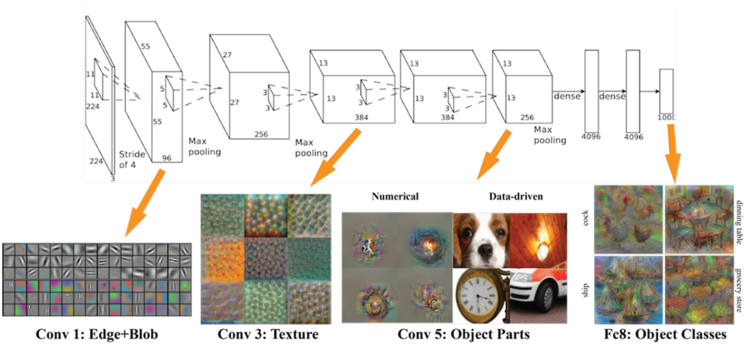
Deep representation - intuition



Bengio, "Learning Deep Architectures for AI", 2009

Ong & Walder & Webers
Data61 | CSIRO
The Australian National University

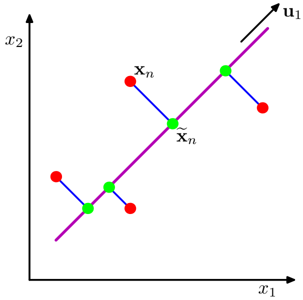
Deep representation - practice



AlexNet / VGG-F network visualized by mNeuron.

Recall: PCA

- Idea: Linearly project the data points onto a lower dimensional subspace such that
  - the variance of the projected data is maximised, or
  - the distortion error from the projection is minimised.
- Both formulation lead to the same result.
- Need to find the lower dimensional subspace, called the principal subspace.



Multiple PCA layers? - linear transforms

- Principle Component Analysis is a linear transformation (because it is a projection)
- The composite of two linear transformations is linear
- Linear transformations $M : \mathbb{R}^m \to \mathbb{R}^n$ are matrices
- Let S and T be matrices of appropriate dimension such that ST is defined

$$ST(X + X') = ST(X) + ST(X')$$

- Similarly for multiplication with a scalar

$\Rightarrow$ multiple PCA layers pointless

Multiple PCA layers? - projection

- Let $X^T X = U \Lambda U^T$ be the eigenvalue decomposition of the covariance matrix (what is assumed about the mean?).
- Define U_k to be the matrix of the first k columns of U, for the k largest eigenvalues. Define Λ_k similarly
- Consider the features formed by projecting onto the principal components

$$Z = X U_k$$

- We perform PCA a second time, $Z^T Z = V \Lambda_Z V^T$.
- By the definition of Z and $X^T X$, and the orthogonality of U

$$Z^T Z = (X U_k)^T (X U_k) = U_k^T X^T X U_k = U_k^T U \Lambda U^T U_k = \Lambda_k$$

- Hence $\Lambda_Z = \Lambda_k$ and V is the identity, therefore the second PCA has no effect

$\Rightarrow$ again, multiple PCA layers pointless

Autoencoder

- An autoencoder is trained to encode the input x into some representation $c(x)$ so that the input can be reconstructed from that representation
- the target output of the autoencoder is the autoencoder input itself
- With one linear hidden layer and the mean squared error criterion, the k hidden units learn to project the input in the span of the first k principal components of the data
- If the hidden layer is nonlinear, the autoencoder behaves differently from PCA, with the ability to capture multimodal aspects of the input distribution
- Let f be the decoder. We want to minimise the reconstruction error

$$\sum_{n=1}^{N} \ell\left(x_n, f(c(x_n))\right)$$

Cost function

- Recall: $f(c(x))$ is the reconstruction produced by the network
- Minimisation of the negative log likelihood of the reconstruction, given the encoding $c(x)$

$$\text{RE} = -\log P(x|c(x))$$

- If $x|c(x)$ is Gaussian, we recover the familiar squared error
- If the inputs x_i are either binary or considered to be binomial probabilities, then the loss function would be the cross entropy

$$-\log P(x|c(x)) = -x_i \log f_i(c(x)) + (1-x_i)\log(1-f_i(c(x)))$$

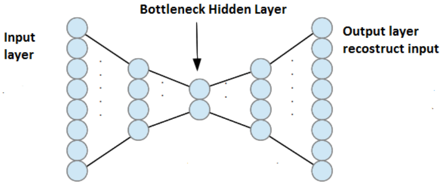
where $f_i(\cdot)$ is the i^{th} component of the decoder

Undercomplete Autoencoder

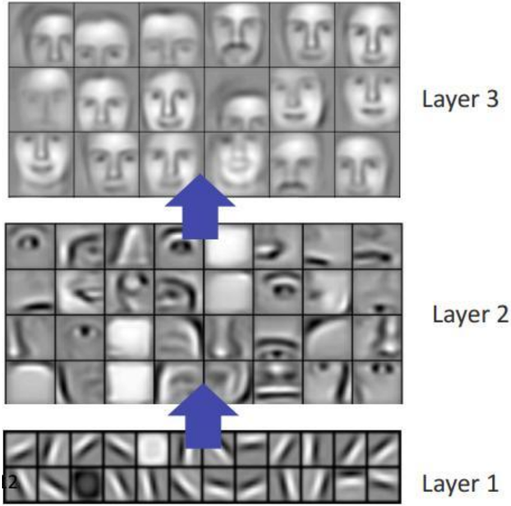
- Consider a small number of hidden units.
- $c(x)$ is viewed as a lossy compression of x
- Cannot have small loss for all x, so focus on training examples
- Hope code $c(x)$ is a distributed representation that captures the main factors of variation in the data

Stacking autoencoders

- Let c_j and f_j be the encoder and corresponding decoder of the j^{th} layer
- Let z_j be the representation after the encoder c_j
- We can define multiple layers of autoencoders recursively.
- For example, let $z_1 = c_1(x)$, and $z_2 = c_2(z_1)$, the corresponding decoding is given by $f_1(f_2(z_2))$
- Because of non-linear activation functions, the latent feature z_2 can capture more complex patterns than z_1.



Higher level image features - faces



codingplayground.blogspot.com

Pre-training supervised neural networks

- Latent features z_j in layer j can capture high level patterns

$$z_j = c_j(c_{j-1}(\cdots c_2(c_1(x))\cdots))$$

- These features may also be useful for supervised learning tasks.
- In contrast to the feed forward network, the features z_j are constructed in an unsupervised fashion.
- Discard the decoding layers, and directly use z_j with a supervised training method, such as logistic regression.
- Various such pre-trained networks are available on-line, e.g VGG-19.

Xavier Initialisation / ReLU

- Layer-wise unsupervised pre-training facilitates learning by extracting useful features for subsequent supervised backprop.
- Pre-training also avoids saturation (large magnitude arguments to, say, sigmoidal units).
- Simpler Xavier initialization can also avoid saturation.
- Let the inputs $x_i \sim \mathcal{N}(0,1)$, weights $w_i \sim \mathcal{N}(0,\sigma^2)$ and activation $z = \sum_{i=1}^m x_i w_i$. Then:

$$\mathrm{VAR}[z] = \mathbb{E}[(z - \mathbb{E}[z])^2] = \mathbb{E}[z^2] = \mathbb{E}[(\sum_{i=1}^m x_i w_i)^2]$$
$$= \sum_{i=1}^m \mathbb{E}[(x_i w_i)^2] = \sum_{i=1}^m \mathbb{E}[x_i^2]\mathbb{E}[w_i^2] = m\sigma^2.$$

- So we set $\sigma = 1/\sqrt{m}$ to have “nice” activations.
- Similarly for subsequent layers in the network.
- ReLU activations $h(x) = \max(x, 0)$ also help in practice.

Higher dimensional hidden layer

- if there is no other constraint, then an autoencoder with d-dimensional input and an encoding of dimension at least d could potentially just learn the identity function
- Avoid by:
  - Regularisation
  - Early stopping of stochastic gradient descent
  - Add noise in the encoding
  - Sparsity constraint on code $c(x)$.

Denoising autoencoder

- Add noise to input, keeping perfect example as output
- Autoencoder tries to:
  1. preserve information of input
  2. undo stochastic corruption process
- Reconstruction log likelihood

$$-\log P(x|c(\hat{x}))$$

where x noise free, $\hat{x}$ corrupted

Image denoising

- Images with Gaussian noise added.

- Denoised using Stacked Sparse Denoising Autoencoder

Images from Xie et. al. NIPS 2012

Inpainting - 1

Free a bird

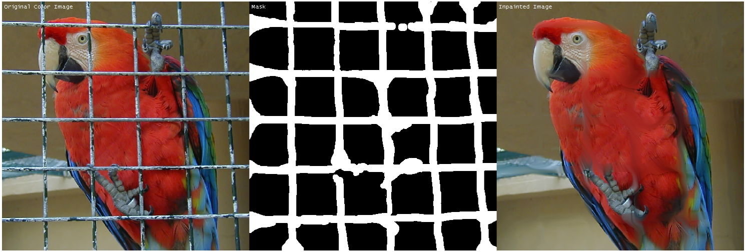


Image from `http://cimg.eu/greycstoration/demonstration.shtml`

Inpainting - 2

Undo text over image

Image from Bach et. al, ICCV tutorial 2009

Recall: Basis functions

- For fixed basis functions $\phi(x)$, we use domain knowledge for encoding features
- Neural networks use data to learn a set of transformations. $\phi_i(x)$ is the i^{th} component of the feature vector, and is learned by the network.
- The transformations $\phi_i(\cdot)$ for a particular dataset may no longer be orthogonal, and furthermore may be minor variations of each other.
- We collect all the transformed features into a matrix Φ.

Sparse representations

- Idea: Have many hidden nodes, but only a few active for a particular code $c(x)$.
- Student t prior on codes
- ℓ_1 penalty on coefficients α
  - Given bases in matrix Φ, look for codes by choosing α such that input signal x is reconstructed with low ℓ_2 reconstruction error, while w is sparse

$$\min_{\alpha} \sum_{n=1}^{N} \frac{1}{2} \|x_n - \Phi \alpha_n\|_2^2 + \lambda \|\alpha\|_1$$

  - Φ is overcomplete, no longer orthogonal
  - Sparse $\Rightarrow$ small number of non-zero α_i.
  - Exact recovery under certain conditions (coherence): $\ell_1 \rightarrow \ell_0$.
  - ℓ_1 regulariser $\sim$ Laplace prior $p(\alpha_i) = \frac{\lambda}{2} \exp(-\lambda|\alpha_i|)$.

The image denoising problem

$$\underbrace{y}_{\text{measurements}} = \underbrace{x_{orig}}_{\text{original image}} + \underbrace{w}_{\text{noise}}$$

Sparsity assumption

- Only have noisy measurements

$$\underbrace{y}_{\text{measurements}} = \underbrace{x_{orig}}_{\text{original image}} + \underbrace{w}_{\text{noise}}$$

- Given $\Phi \in \mathbb{R}^{m \times p}$, find α such that

$$\|\alpha\|_0 \quad \text{is small} \quad \text{for} \quad x \approx \Phi\alpha$$

  where $\|\cdot\|_0$ is the number of non-zero elements of α.
- Φ is not necessarily features constructed from training data.
- Minimise reconstruction error

$$\min_{\alpha} \sum_{n=1}^{N} \frac{1}{2}\|x_n - \Phi\alpha_n\|_2^2 + \lambda\|\alpha\|_0$$

Convex relaxation

- Want to minimise number of components

$$\min_{\alpha} \sum_{n=1}^{N} \frac{1}{2} \|x_n - \Phi\alpha_n\|_2^2 + \lambda\|\alpha\|_0$$

  but $\|\cdot\|_0$ is hard to optimise
- Relax to a convex norm

$$\min_{\alpha} \sum_{n=1}^{N} \frac{1}{2} \|x_n - \Phi\alpha_n\|_2^2 + \lambda\|\alpha\|_1$$

  where $\|\alpha\|_1 = \sum_n |\alpha_n|$.
- In some settings does minimisation with ℓ_1 regularisation give the same solution as minimisation with ℓ_0 regularisation (exact recovery)?

Mutual coherence

- Expect to be ok when columns of Φ “not too parallel”
- Assume columns of Φ are normalised to unit norm
- Let $K = \Phi\Phi^T$ be the Gram matrix, then $K(i,j)$ is the value of the inner product between ϕ_i and ϕ_j.
- Define the mutual coherence

$$M = M(\Phi) = \max_{i \neq j} |K(i,j)|$$

- If we have an orthogonal basis, then Φ is an orthogonal matrix, hence $K(i,j) = 0$ when $i \neq j$.
- However, if we have very similar columns, then $M \approx 1$.

Exact recovery conditions

- If a minimiser of the true ℓ_0 problem, α^* satisfies

$$\|\alpha^*\|_0 < \frac{1}{M}$$

then it is the unique sparsest solution.

- If α^* satisfies the stronger condition

$$\|\alpha^*\|_0 < \frac{1}{2}\left(1 + \frac{1}{M}\right)$$

then the minimiser of the ℓ_1 relaxation has the same sparsity pattern as α^*.

References

- Yoshua Bengio, "Learning Deep Architectures for AI", Foundations and Trends in Machine Learning, 2009
- `http://deeplearning.net/tutorial/`
- `http://www.deeplearningbook.org/contents/autoencoders.html`
- Fuchs, "On Sparse Representations in Arbitrary Redundant Bases", IEEE Trans. Info. Theory, 2004
- Xavier Glorot and Yoshua Bengio, "Understanding the difficulty of training deep feedforward neural networks", 2010.

Ong & Walder & Webers
Data61 | CSIRO
The Australian National University