

From Linear Regression to Deep Neural Networks to Segmentation

Lucas C Parra



Linear Regression

X

Model

Error



Cost function
$$E(w_1, w_0) = \sum_n ({}^n e)^2$$

Mean square error $\hat{w}_1, \hat{w}_0 = \underset{w_1, w_0}{\operatorname{argmin}} E(w_1, w_0)$

 $\hat{y} = \mathbf{W}_1 \mathbf{x} + \mathbf{W}_0$

 $e = \hat{y} - y$

 $(^{n}x, ^{n}y), n=1...N$

<i>w</i> ₁		(\hat{w}_1, \hat{w}_0)
	w ₀	2

Revisiting segmentation by fitting the background

Linear model with quadratic error

$$E(\boldsymbol{w}) = \sum_{n} ({}^{n}\boldsymbol{y} - \boldsymbol{w}^{T} \cdot {}^{n}\boldsymbol{x})^{2}$$

has closed from solution:

$$\hat{\boldsymbol{w}} = \left(\sum_{n} {}^{n}\boldsymbol{x} \cdot {}^{n}\boldsymbol{x}^{T}\right)^{-1} \cdot \left(\sum_{n} {}^{n}\boldsymbol{x} \cdot {}^{n}\boldsymbol{y}\right)$$
$$= R_{xx}^{-1} \cdot R_{xy} = \boldsymbol{x} \setminus \boldsymbol{y}$$

Notice that subtraction and thresholding is a linear operation followed by nonlinearity

```
>> [X,Y] = meshgrid(1:size(img,2),1:size(img,1));
>> img = img - mycurvefit(img,X,Y); % linear prediction from X,Y
>> img = img > graythresh(img); % nonlinearity
```

Making position of the input also a feature to predict the output is called "position encoding" in machine learning.

```
function Zest = mycurvefit(Z,X,Y)
% Zest = mycurvefit(Z) fit Z to be approximated by
% Zest=w1+w2*X+w3*Y+w4*Y^2 in a least squares sense.
dims = size(Z); [X,Y] = meshgrid(1:dims(2),1:dims(1));
woptimal = [ones(size(Z(:))) X(:) Y(:) Y(:).^2]\Z(:);
Zest = mycurve(woptimal,X,Y);
```

```
function Zest = mycurve(p,X,Y);
Zest = w(1)+w(2)*X+w(3)*Y+w(4)*Y.^2;
```

This segmentation code could be called a "single layer dense network with position encoding".

Revisiting segmentation by fitting the background city College of New York intensity and thresholding:



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Logistic Regression

Data

Model

Sigmoid

 $(^{n}x, ^{n}y), n=1...N$ $\hat{y} = f(w_{1}x + w_{0})$ $\hat{y} = f(x) = \frac{\exp(x)}{1 + \exp(x)}$

Cost $c = -y \log \hat{y} - (1-y) \log (1-\hat{y})$ (binary cross entropy)

Cost function

 $E(w_1, w_0) = \sum_n {}^n c$

Learning

$$\hat{w}_1, \hat{w}_0 = \operatorname{argmin}_{w_1, w_0} E(w_1, w_0)$$







Data

$$({}^{n}x_{1}...{}^{n}x_{D_{x}},{}^{n}y_{1}...{}^{n}y_{D_{y}}), n=1...N$$

Model



Softmax

Think of *x_i* as the strength of evidence for class *i*

Cost $c_i = -y_i \log \hat{y}_i$ (categorical cross entropy)

Cost function

$$E(w_{ij}) = \sum_{n} \sum_{i} {}^{n} c_{i}$$

Learning

$$\hat{w}_{ij} = \underset{w_{ij}}{argmin} E(w_{ij})$$

Softmax





"Dense network layer"



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Gradient Descent

$$\hat{w}_{ij} = \underset{w_{ij}}{argmin} E(w_{ij})$$

Gradient descent

$$\Delta \mathbf{w}_{ij} = -\lambda \frac{dE}{dw_{ij}}$$

Stochastic Gradient descent for sample n

$$\Delta^n w_{ij} = -\lambda \frac{d({}^n e)}{dw_{ij}}$$





Multilayer Perceptron

Layers l=0...LModel $a_i^l = f_i^l (\sum_j w_{ij}^l a_j^{l-1}) \qquad a_i^0 = x_i$ ReLU a=max(0,x)

Gradient back propagation

$$g_{j}^{l-1} = \sum_{i} f_{i}^{l} w_{ij}^{l} g_{i}^{l} \qquad g_{i}^{L} = 2e$$

Cost function

$$E = \sum_{n} \sum_{i} |{}^{n}e_{i}|^{2}$$

Stochastic Gradient $\Delta w_{ij}^{l} = -\lambda f_{i}^{l} g_{i}^{l} a_{j}^{l-1}$ descent:



"3 dense network layers" 8



Example: NIST digit classification

Osvaldo Velarde:

Introduce google colab.

Present example in python from

"Deep Learning with Python" Book by François Chollet, 2nd edition, Manning.

Chapter 2, MNIST digit classification with 2 layer dense network.

Convolutional Neural Network (CNN)

1.1

Weights are shift invariant:

$$w_{ij} = w_{i-j} = w_k \qquad w_1 w_2 w_3$$

el $a_i^l = f(\sum_k w_k a_{i-k}^{l-1})$

Model

i.e. all units have the same weights; weights are "tied"

Gradient update is summed over all "tied" weights*

$$\Delta w_k^l = -\lambda \sum_i f_i^l g_i^l a_{i-k}^{l-1}$$

* this is true for any kind of weight symmetry that shares weights



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"convolution layer"

Pooling

Reduce resolution by taking the maximum or mean, e.g.

 $a_i^l = max(a_i^{l-1}, a_{i-1}^{l-1})$

The gradient only propagates to the units that contribute to the pooled value, e.g. gradient is zero for units that were not selected in the maximum.

Other forms of reducing resolution with convolution:

Stride – skip intermediate pixels; is the same as weighted average pooling. Downsampling – same as weighted average pooling but with predefined weights. "valid" – reduce size at the boundary, bonus: avoids edge artifacts.



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"pooling layer"





Deep CNN

Layers can be stacked up into deep networks. With CNN, typically decreasing spatial resolution while increasingly number of "channels"





CNN features

Increasing complexity of features in successive layers.





Deep network tricks

Equations for activation, gradients, and weight updates have all been automated, e.g. in TensorFlow or Pytorch. All that is needed is to define the network architecture, e.g. in Keras.

Deep networks with many layers have a number of <u>problems</u>, but also remarkably effective heuristic solutions (some keywords for independent study):

Repeated multiplication with f' causes vanishing gradients in deep layers. Solutions:

- ReLU non-linearity
- Batch normalization

Repeated mixing with $\sum_{i} w_{ii}$ causes <u>diluted gradients</u> in deep layers (my wording). Solutions:

- Residual connections
- Max pooling
- Attention gating

With millions of free parameters <u>over-training</u> is the norm. Solutions:

- Tying weights (symmetry)
- Dropout
- Early stopping
- Self supervised learning
- Transfer learning



Segmentation with UNets



Lucas Parra Down and up-sampling



Downsampling by 2: low-pass and then take every other sample, e.g. "mean pooling" with "stride" 2. Umsampling: insert zeros and then filter with point spread function. "Transpose convolution"

Constant weights $\bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{j} \bigvee_{i} \bigvee_{i}$



Linear weight



Example: Neuron segmentation

Osvaldo Velarde

Present example of UNet in colab for segmenting 2D phase contrast images of neurons.

Lucas Parra Down and up-sampling

Constant weights



Original and recovred

20

40

0.2

0.1

-0.1

-0.2

0





This is TensorFlow default initialization and tends to cause grid-artifacts. Needs to "learn" to avoid them.



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Optimal without need to learn. Weights can be set fixed.