More on Training Deep Neural Networks

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Introduction to Deep Learning

Overview

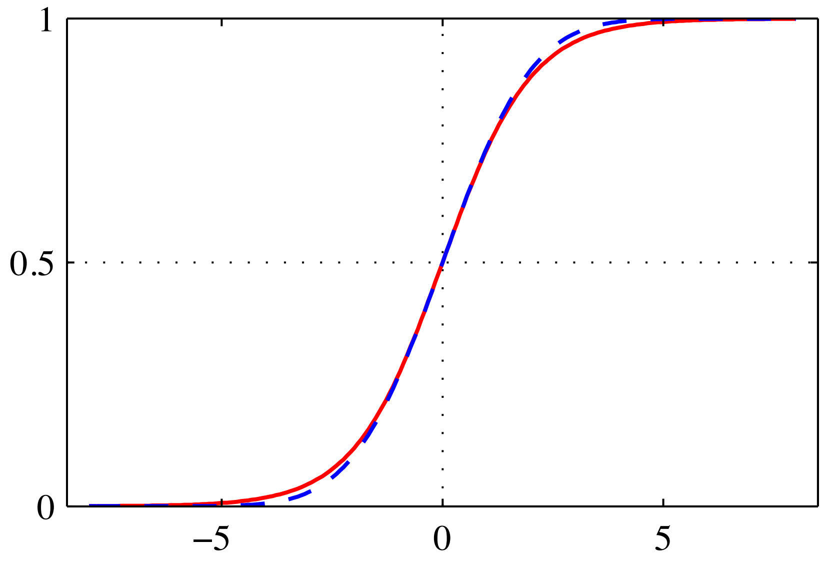
- Rectified Linear Units
- Regularization
  - Dropout
  - Norm Constraint
- Adapting Step Sizes
- Batch Normalization
- Babysitting the Training Process

Rectified Linear Units

A New Activation Function

Vanishing Gradients

- Activation functions that approximate step functions have small gradients outside their center.
- This is exacerbated by backpropagation across many layers: according to the chain rule, gradients are multiplied.
  - Problem for deep learning, recurrent neural networks

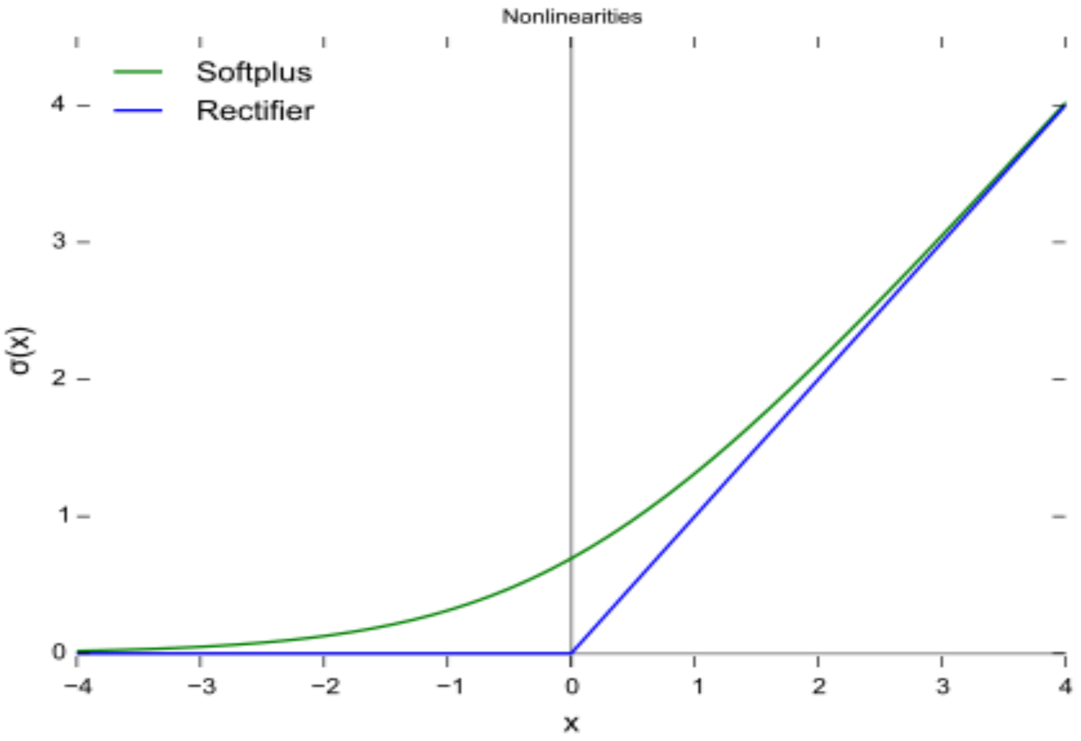


Problems with Sigmoid Activation Function

- Dense: typically all units are active for any given input.
- Vanishing gradient: as number of layers increase, the error derivative for each goes to 0.
- ➢ Do not use sigmoid for hidden nodes
- Hyperbolic tangent is better than sigmoid
- Usually Rectified Linear activation is best
- See tensor playground demo

Rectified Linear Unit

- $f(x) = \max(0,x)$
- Gradient is trivial.



CC0, https://en.wikipedia.org/w/index.php?curid=48817276

Co-Adaptation and Regularization

Local Minima and Local Gradients

- How does a neural network get stuck in a local minimum?
- Many reasons, but key phenomenon is that gradients are directions for single weights <u>not sets of weights</u>.
  - Definition of gradient for *w*: *fix all other weights, consider depending of error function E on w in isolation*.
- Example: XOR
  - Moving weight for single feature does not help, need to move weight for both.

Local Minima and Co-Adaptation

- Because weights are changed one at a time, a bad value for w_1 can lead to bad values for w_2.
    - See UBC tool demo neural.jar
- This is called <u>co-adaptation</u>.
- Related to overfitting.
- Toy Example:

	w_1	w_2
Optimal Value	1	1
Local Minimum	8	-6

A common symptom of co-adaptation and overfitting are excessively large weight magnitudes. How can we address this?

Regularization

- Add a term to loss function that penalizes large weights
  minimize $E(\mathbf{w}) + \lambda||\mathbf{w}||$

- Need to set the trade-off parameter λ

- Very common in machine learning
- The norm constraint: Fix the length $||\mathbf{w}||$ of each weight vector to be less than a constant.

Dropout

- Model Averaging comes to Neural Nets
- Averaging Models is a good idea
  - See boosting

Dropout in Neural Nets

1. Stochastic gradient descent: Cycle through each case.
2. For each case, randomly drop out some neurons.
   1. Independently with probability p, e.g. 0.5.
   2. Train only the weights for the remaining neurons.
3. After training, multiply the weights by p. Intuition:
   1. A kind of average over the neural net for each case.
   2. If $p = 0.5$, twice as many hidden units are present as during training.

   Typically also use the norm constraint.

Dropout Picture

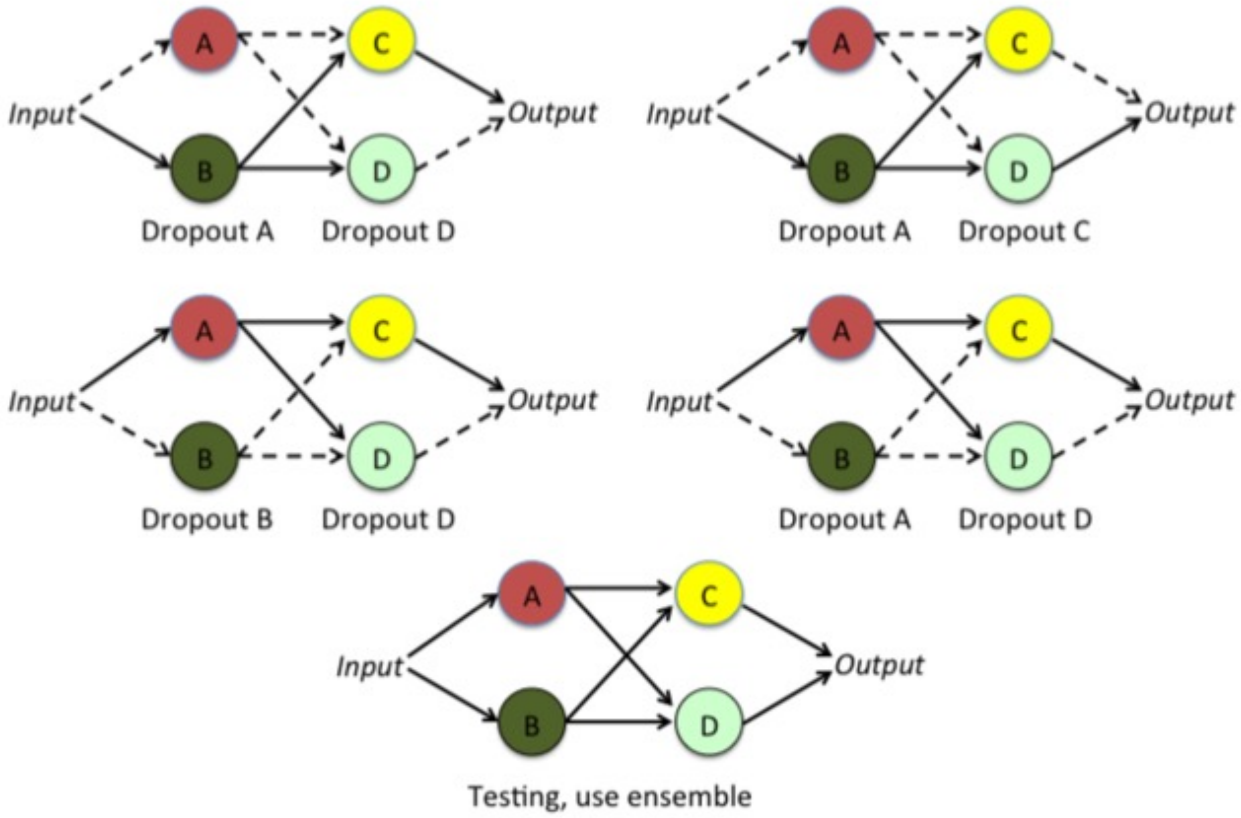


Illustration of dropout when there are 2 hidden layers and 2 hidden neurons.

https://medium.com/@vivek.yadav/why-dropouts-prevent-overfitting-in-deep-neural-networks-937e2543a701

Step Size Adaptation

See normalization survey on canvas

Gradients of Gradients

- Remember the driving example: Want to slow down getting close to the goal.
  - Especially if gradients flip sign (left-right-left-right).
  - ➢ Fast change in gradients $\longrightarrow$ smaller steps.
- Formal Idea: Make step size the inverse of 2nd-order derivative.
- Newton Raphson Update Rule:
  $x := x - \eta f'(x)/f''(x)$

Analyzing Gradients

- Newton—Raphson is good
- But for many (millions) of parameters, cannot feasibly get all the 2nd-order gradients (the Hessian).
  - Nor can we invert the Hessian matrix.
- Instead use the trends in gradient sequence as estimates of curvature.
- Many developments of this basic idea.
  - Typically user specifies initial learning rate and method adapts as training proceeds
  - We'll look at the ADAM method (Adaptive Moment Estimation).

ADAM Intuitions

- Input: sequence of observed gradients $g_1, \ldots, g_t$

1. Divide learning rate by observed variance/standard deviation.
   - Variance replaces curvature in Newton-Raphson
2. Update with average of gradients seen so far (not current gradient)
   - Intuitively, like the momentum of a moving object

Estimate Gradient Moments

- Input: sequence of observed gradients $g_1, \ldots, g_t$
- Output: estimate *exponentially discounted* gradient average, (uncentered) standard deviation
- Decay factor β_1 for average. E.g. for $t = 3$, $\beta_1 = 0.9$
  - $m_3 = 0.9 \times 0.9 \times (1-0.9)\, g_1 + 0.9 \times (1-0.9)\, g_2 + (1-0.9)\, g_3$
  - Common idea for time series
- Incremental Running Average Update:
  $m_t = \beta_1\, m_{t-1} + (1 - \beta_1)\, g_t$
- Similar for variance with another decay factor
  $v_t = \beta_2\, v_{t-1} + (1 - \beta_2)\, (g_t)^2$

Update Formula

- Bias correction:

  $m_t := m_t /(1 - [\beta_1]^t)$

  $v_t := v_t /(1 - [\beta_2]^t)$

- $w_t := w_{t-1} - \eta\, \underbrace{m_t}_{\text{update by (estimated) average gradient}} / [\underbrace{(v_t)^{1/2}}_{\text{Divide update by standard deviation}} + \varepsilon)]$

update by (estimated)
average gradient

Divide update
by standard deviation

Batch Normalization

Normalization Survey on Canvas

High-level Intuition

- From the point of view of hidden layers inside a deep network:
  output activation of previous layer = input "data"

➢ whatever properties we want in input data ➔ properties we want in output activations

- one nice input data property was normalization
  - means and variances on the same scale
  - e.g. all data dimensions on the same scale (see preprocessing section)

Benefits of Normalized Activations

- avoid saturation
- less dependence on initial weight values
- some regularization: large values scaled back

Normalization Algorithm

For minibatch $\mathbf{x}_1,..\mathbf{x}_\mathrm{m}$ of data points

For each node x^i

1. Find the activation values $x^i{}_j,.., x^i{}_m$ for each data point
2. Normalize the activation values:

$$\mathrm{mean}_i := 1/m \sum_{j=0}^{m} x_j^i$$

$$\mathrm{var}_i := 1/m \sum_{j=0}^{m} (x_j^i - \mathrm{mean}_i)^2$$

$$\hat{x}_i := \frac{x_i - \mathrm{mean}_i}{\sqrt{\mathrm{var}_i + \varepsilon}}$$

3. Scale and shift: $y_i := \gamma \hat{x}_i + \beta$

   where γ,β are learned during backpropagation

Conclusion

- Many tips and tricks to try, little theory or guarantees
- For output nodes:
  - Use sigmoid + cross-entropy for classification
  - Use linear + least-squares for regression
- For hidden nodes:
  - Don’t use sigmoid
  - Relu is good default
  - Can try hyperbolic tangent
- Adapting the step size is a good idea
- Drop out and batch normalization sometimes help
- Regularization is a good idea (more next time)