Neural networks

COMS 4771 Fall 2019

Overview

- Structure and power of neural networks
- Backpropagation
- Practical issues
- Convolutions

Parametric featurizations I

- So far: features ($\boldsymbol{x}$ or $\varphi(\boldsymbol{x})$) are fixed during training
  - Consider a (small) collection of feature transformations φ
  - Select φ via cross-validation – outside of normal training
- "Deep learning" approach:
  - Use φ with many tunable parameters
  - Optimize parameters of φ during normal training process

Parametric featurizations II

- *Neural network*: parameterization for function $f\colon \mathbb{R}^d \to \mathbb{R}$
  - $f(\boldsymbol{x}) = \varphi(\boldsymbol{x})^{\mathsf{T}}\boldsymbol{w}$
  - Parameters include both $\boldsymbol{w}$ and parameters of φ
  - Varying parameters of φ allows f to be essentially any function!
  - Major challenge: optimization (a lot of tricks to make it work)

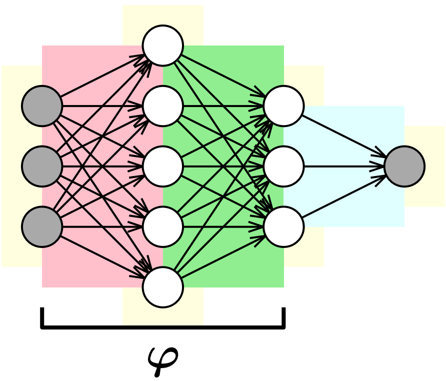


Figure 1: Neural network

Feedforward neural network

- *Architecture* of a *feedforward neural network*
  - Directed acyclic graph $G = (V, E)$
  - One *source* node (vertex) per input, one *sink* node per output
  - Other nodes are *hidden units*
  - Each edge $(u, v) \in E$ has a *weight parameter* $w_{u,v} \in \mathbb{R}$
  - *Value* h_v of node v given values of parents is

$$h_v := \sigma_v(z_v), \quad z_v := \sum_{u \in V : (u,v) \in E} w_{u,v} \cdot h_u.$$

    - $\sigma_v : \mathbb{R} \to \mathbb{R}$ is the *activation function* (e.g., sigmoid)

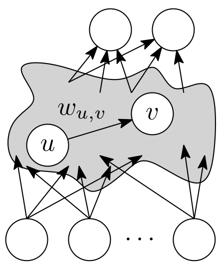


Figure 2: Feedforward neural network architecture

Standard layered architectures

- Standard architecture arranges nodes into sequence of L *layers*
- Edges only go from one layer to the next
- Can write function using matrices of weight parameters

$$f(\boldsymbol{x}) = \sigma_L(\boldsymbol{W}_L \sigma_{L-1}(\cdots \sigma_1(\boldsymbol{W}_1 \boldsymbol{x}) \cdots))$$

  - d_ℓ nodes in layer ℓ; $\boldsymbol{W}_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$ are weight parameters
  - Activation function $\sigma_\ell : \mathbb{R} \to \mathbb{R}$ is applied coordinate-wise to input
- Often also include "bias" parameters $\boldsymbol{b}_\ell \in \mathbb{R}^{d_\ell}$

$$f(\boldsymbol{x}) = \sigma_L(\boldsymbol{b}_L + \boldsymbol{W}_L \sigma_{L-1}(\cdots \sigma_1(\boldsymbol{b}_1 + \boldsymbol{W}_1 \boldsymbol{x}) \cdots))$$

- Tunable parameters: $\boldsymbol{\theta} = (\boldsymbol{W}_1, \boldsymbol{b}_1, \ldots, \boldsymbol{W}_L, \boldsymbol{b}_L)$

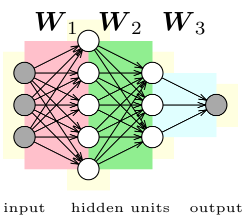


Figure 3: Standard feedforward architecture

Well-known activation functions

- *Heaviside*: $\sigma(z) = \mathbb{1}_{\{z \geq 0\}}$
  - Popular in the 1940s; also called *step function*
- *Sigmoid* (from logistic regression): $\sigma(z) = 1/(1 + e^{-z})$
  - Popular since 1970s
- *Hyperbolic tangent*: $\sigma(z) = \tanh(z)$
  - Similar to sigmoid, but range is $(-1, 1)$ rather than $(0, 1)$
- *Rectified Linear Unit* (*ReLU*): $\sigma(z) = \max\{0, z\}$
  - Popular since 2012
- *Identity*: $\sigma(z) = z$
  - Popular with luddites
- *Softmax*: $\sigma(\boldsymbol{v})_i = \exp(v_i) / \sum_j \exp(v_j)$
  - Special vector-valued activation function
  - Popular for final layer in multi-class classification

Power of non-linear activations

- What happens if every activation function is linear/affine?

Necessity of multiple layers

- Suppose only have input and output layers, so function f is

$$f(\boldsymbol{x}) = \sigma(b + \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x})$$

where $b \in \mathbb{R}$ and $\boldsymbol{w} \in \mathbb{R}^d$ (so $\boldsymbol{w}^{\mathsf{T}} \in \mathbb{R}^{1\times d}$)
- If σ is monotone (e.g., Heaviside, sigmoid, hyperbolic tangent, ReLU, identity), then f has same limitations as a linear/affine classifier

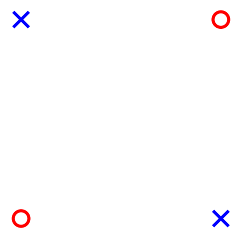


Figure 4: XOR problem

Neural network approximation theorems

- **Theorem** (Cybenko, 1989; Hornik, Stinchcombe, & White, 1989): For any continuous function $f\colon \mathbb{R}^d \to \mathbb{R}$ and any $\varepsilon > 0$, there is a two-layer neural network (with parameters $\boldsymbol{\theta} = (\boldsymbol{W}_1, \boldsymbol{b}_1, \boldsymbol{w}_2)$) s.t.

$$\max_{\boldsymbol{x}\in[0,1]^d} |f(\boldsymbol{x}) - \boldsymbol{w}_2^{\mathsf{T}}\sigma_1(\boldsymbol{b}_1 + \boldsymbol{W}_1\boldsymbol{x})| < \varepsilon.$$

Here, σ_1 can be any non-linear activation function from above.

- Many caveats
  - "Width" (number of hidden units) may need to be very large
  - Does not tell us how to find the network
  - Does not justify deeper networks

Fitting neural networks to data

- Training data $(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n) \in \mathbb{R}^d \times \mathcal{Y}$
- Fix architecture: $G = (V, E)$ and activation functions
- Plug-in principle: find parameters $\boldsymbol{\theta}$ of neural network $f_{\boldsymbol{\theta}}$ to minimize empirical risk (possibly with a surrogate loss)

$$\widehat{\mathcal{R}}(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i)^2 \qquad \text{regression}$$

$$\widehat{\mathcal{R}}(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\ell_{\log}(-y_i f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)) \qquad \text{binary classification}$$

$$\widehat{\mathcal{R}}(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\ell_{\mathrm{ce}}(\tilde{\boldsymbol{y}}_i, f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)) \qquad \text{multi-class classification}$$

(Could use other surrogate loss functions . . .)
- Typically objective is not convex in parameters $\boldsymbol{\theta}$
- Nevertheless, local search (e.g., SGD) often works well!

Backpropagation

- *Backpropagation (backprop)*: Algorithm for computing partial derivatives wrt weights in a feedforward neural network
  - Clever organization of partial derivative computations with *chain rule*
  - Use in combination with gradient descent, SGD, etc.
- Consider loss on a single example $(\boldsymbol{x}, y)$, written $J := \ell(y, f_{\boldsymbol{\theta}}(\boldsymbol{x}))$
- Goal: compute $\frac{\partial J}{\partial w_{u,v}}$ for every edge $(u, v) \in E$
- Initial step of backprop: *forward propagation*
  - Compute z_v's and h_v's for every node $v \in V$
  - Running time: linear in size of network
- Rest of backprop also just requires time linear in size of network!

Derivative of loss with respect to weights

- Let $\hat{y}_1, \hat{y}_2, \ldots$ denote the values at the output nodes.
- Then by chain rule,

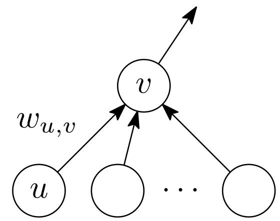
$$\frac{\partial J}{w_{u,v}} = \sum_i \frac{\partial J}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{w_{u,v}}.$$

Derivative of output with respect to weights

- Assume for simplicity there is just a single output, $\hat{y}$
- Chain rule, again:

$$\frac{\partial \hat{y}}{\partial w_{u,v}} = \frac{\partial \hat{y}}{\partial h_v} \cdot \frac{\partial h_v}{\partial w_{u,v}}$$

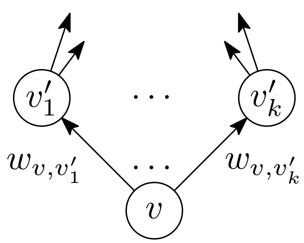
- First term: trickier; we'll handle later
- Second term:



Derivative of output with respect to hidden units

- Compute $\frac{\partial \hat{y}}{\partial h_v}$ for all vertices in decreasing order of layer number
- If v is not the output node, then by chain rule (yet again),

$$\frac{\partial \hat{y}}{\partial h_v} = \sum_{v' : (v,v') \in E} \frac{\partial \hat{y}}{\partial h_{v'}} \cdot \frac{\partial h_{v'}}{\partial h_v}$$



Example: chain graph I

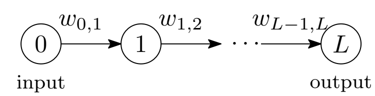


Figure 5: Chain graph; assume same activation σ in every layer

- Parameters $\boldsymbol{\theta} = (w_{0,1}, w_{1,2}, \ldots, w_{L-1,L})$
- Fix input value $x \in \mathbb{R}$; what is $\frac{\partial h_L}{\partial w_{i-1,i}}$ for $i = 1, \ldots, L$?
- Forward propagation:
  - $h_0 := x$
  - For $i = 1, 2, \ldots, L$:

$$z_i := w_{i-1,i} h_{i-1}$$
$$h_i := \sigma(z_i)$$

Example: chain graph II

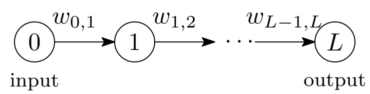


Figure 6: Chain graph; assume same activation σ in every layer

- Backprop:
  - For $i = L, L-1, \ldots, 1$:

$$\frac{\partial h_L}{\partial h_i} := \begin{cases} 1 & \text{if } i = L \\ \frac{\partial h_L}{\partial h_{i+1}} \cdot \sigma'(z_{i+1}) w_{i,i+1} & \text{if } i < L \end{cases}$$

$$\frac{\partial h_L}{\partial w_{i-1,i}} := \frac{\partial h_L}{\partial h_i} \cdot \sigma'(z_i) h_{i-1}$$

Practical issues I: Initialization

- Ensure inputs are *standardized*: every feature has zero mean and unit variance (wrt training data)
- Initialize weights randomly for gradient descent / SGD

Practical issues II: Architecture choice

- Architecture can be regarded as a "hyperparameter"
- Optimization-inspired architecture choice
  - With wide enough network, can get training error rate zero
  - Use the smallest network that lets you get zero training error rate
  - Then add regularization term to objective (e.g., sum of squares of weights), and optimize the regularized ERM objective
- Entire research communities are trying to figure out good architectures for their problems

Convolutional nets

- Neural networks with *convolutional layers*
  - Useful when inputs have locality structure
  - Sequential structure (e.g., speech waveform)
  - 2D grid structure (e.g., image)
  - $\ldots$
- Weight matrix $\boldsymbol{W}_\ell$ is highly-structured
  - Determined by a small *filter*
  - Time to compute $\boldsymbol{W}_\ell \boldsymbol{h}_{\ell-1}$ is typically $\ll d_\ell \times d_{\ell-1}$ (e.g., closer to $\max\{d_\ell, d_{\ell-1}\}$)

Convolutions I

- Convolution of two continuous functions: $h := f * g$

$$h(x) = \int_{-\infty}^{+\infty} f(y) g(x-y)\,\mathrm{d}y$$

- If $f(x) = 0$ for $x \notin [-w, +w]$, then

$$h(x) = \int_{-w}^{+w} f(y) g(x-y)\,\mathrm{d}y$$

  - Replaces $g(x)$ with weighted combination of g at nearby points
- For functions on discrete domain, replace integral with sum

$$h(i) = \sum_{j=-\infty}^{\infty} f(j) g(i-j)$$

Convolutions II

- E.g., suppose only $f(0), f(1), f(2)$ are non-zero, and g is *zero-padded* (in this case, $g(i) = 0$ for $i < 1$ or $i > 5$). Then:

$$\begin{bmatrix} h(1) \\ h(2) \\ h(3) \\ h(4) \\ h(5) \\ h(6) \\ h(7) \end{bmatrix} = \begin{bmatrix} f(0) & 0 & 0 & 0 & 0 \\ f(1) & f(0) & 0 & 0 & 0 \\ f(2) & f(1) & f(0) & 0 & 0 \\ 0 & f(2) & f(1) & f(0) & 0 \\ 0 & 0 & f(2) & f(1) & f(0) \\ 0 & 0 & 0 & f(2) & f(1) \\ 0 & 0 & 0 & 0 & f(2) \end{bmatrix} \begin{bmatrix} g(1) \\ g(2) \\ g(3) \\ g(4) \\ g(5) \end{bmatrix}$$

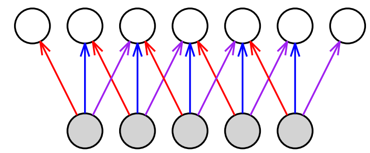


Figure 7: Convolutional layer

2D convolutions I

- Similar for 2D inputs (e.g., images), except now sum over two indices
  - g is the input image
  - f is the filter
  - Lots of variations (e.g., padding, strides, multiple "channels")

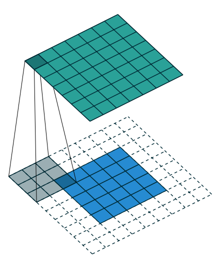


Figure 8: 2D convolution, with padding, no stride

2D convolutions II

- Similar for 2D inputs (e.g., images), except now sum over two indices
  - g is the input image
  - f is the filter
  - Lots of variations (e.g., padding, strides, multiple "channels")

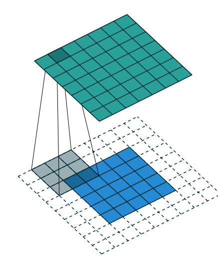


Figure 9: 2D convolution, with padding, no stride

2D convolutions III

- Similar for 2D inputs (e.g., images), except now sum over two indices
  - g is the input image
  - f is the filter
  - Lots of variations (e.g., padding, strides, multiple "channels")

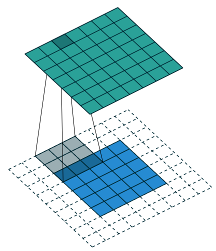


Figure 10: 2D convolution, with padding, no stride

2D convolutions IV

- Similar for 2D inputs (e.g., images), except now sum over two indices
  - g is the input image
  - f is the filter
  - Lots of variations (e.g., padding, strides, multiple "channels")

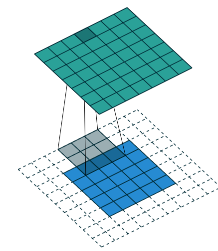


Figure 11: 2D convolution, with padding, no stride

- Use additional layers/activations to down-sample after convolution

Postscript: Tangent model

- Let $f_{\boldsymbol{\theta}} \colon \mathbb{R}^d \to \mathbb{R}$ be a neural network function with parameters $\boldsymbol{\theta} \in \mathbb{R}^p$ (p is total number of parameters)
- Fix $\boldsymbol{x}$, and consider first-order approximation of $f_{\boldsymbol{\theta}}(\boldsymbol{x})$ around $\boldsymbol{\theta} = \boldsymbol{\theta}^{(0)}$:

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) \approx f_{\boldsymbol{\theta}^{(0)}}(\boldsymbol{x}) + \nabla f_{\boldsymbol{\theta}^{(0)}}(\boldsymbol{x})^{\mathsf{T}}(\boldsymbol{\theta} - \boldsymbol{\theta}^{(0)})$$

  Here, ∇ is gradient wrt parameters $\boldsymbol{\theta}$, not wrt input $\boldsymbol{x}$
- Consider feature transformation $\boldsymbol{\varphi}(\boldsymbol{x}) := \nabla f_{\boldsymbol{\theta}^{(0)}}(\boldsymbol{x})$, determined entirely by initial parameters $\boldsymbol{\theta}^{(0)}$
- If the first-order approximation is accurate (i.e., we never consider $\boldsymbol{\theta}$ too far from $\boldsymbol{\theta}^{(0)}$), then back to a linear model (over p features $\boldsymbol{\varphi}(\boldsymbol{x}) \in \mathbb{R}^p$)
  - Called the *tangent model*
- Upshot: To really exploit power of "deep learning", we must be changing parameters a lot during training!