Feature Learning

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Slides based on Lecture 12a from David Rosenberg's course materials

 $\big(\texttt{https://github.com/davidrosenberg/mlcourse} \big)$

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Today's lecture

- Neural networks: huge empirical success but poor theoretical understanding
- Key idea: representation learning
- Optimization: backpropagation + SGD

Overview

Feature engineering

• Learning non-linear models in a linear form:

$$f(x) = w^T \phi(x). \tag{1}$$

- What are possible ϕ 's we have seen?
 - Feature maps that define a kernel, e.g., polynomials of x
 - Feature templates, e.g., x_i AND x_{i-1}
 - Basis functions, e.g., (shallow) decision trees

Decompose the problem

• Example:

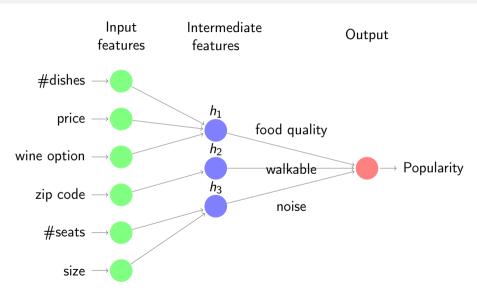
Task Predict popularity of restaurants.

Raw features #dishes, price, wine option, zip code, #seats, size

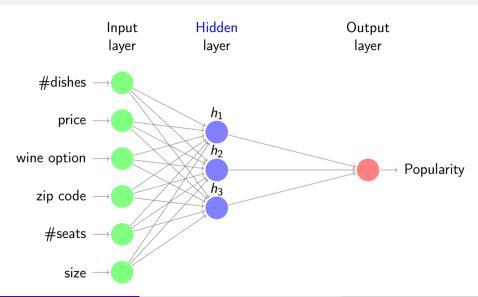
- Decompose into subproblems:
 - $h_1([\#dishes, price, wine option]) = food quality$
 - $h_2([zip code]) = walkable$
 - h₃([#seats, size]) = nosie
- Final *linear* predictor uses **intermediate features** computed by h_i 's:

 $w_1 \cdot \text{food quality} + w_2 \cdot \text{walkable} + w_3 \cdot \text{nosie}$

Predefined subproblems



Learned intermediate features



Neural networks

Key idea: automatically learn the intermediate features.

Feature engineering Manually specify $\phi(x)$ based on domain knowledge and learn the weights:

$$f(x) = \mathbf{w}^T \phi(x). \tag{2}$$

Feature learning Automatically learn both the features (K hidden units) and the weights:

$$h(x) = [h_1(x), \dots, h_K(x)],$$
 (3)

$$f(x) = \mathbf{w}^T h(x) \tag{4}$$

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Activation function

• How should we parametrize h_i 's? Can it be linear?

$$h_i(x) = \sigma(v_i^T x). \tag{5}$$

- σ is the *nonlinear* activation function.
- What might be some activation functions we want to use?
 - sign function? Non-differentiable.
 - · Differentiable approximations: sigmoid functions. S-shaped
 - E.g., logistic function, hyperbolic tangent function.
- Two-layer neural network (one hidden layer and one output layer) with K hidden units:

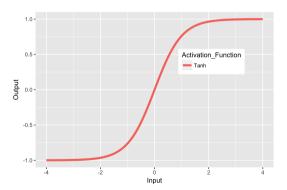
$$f(x) = \sum_{k=1}^{K} w_k h_k(x) = \sum_{k=1}^{K} w_k \sigma(v_k^T x)$$
 (6)

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Activation Functions

• The hyperbolic tangent is a common activation function:

$$\sigma(x) = \tanh(x)$$
.



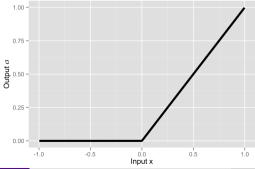
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Activation Functions

• More recently, the rectified linear (ReLU) function has been very popular:

$$\sigma(x) = \max(0, x).$$

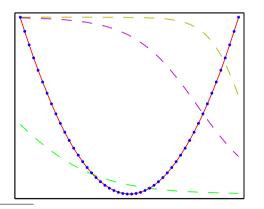
- Much faster to calculate, and to calculate its derivatives.
- Also often seems to work better.



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Approximation Ability: $f(x) = x^2$

- 3 hidden units; tanh activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.

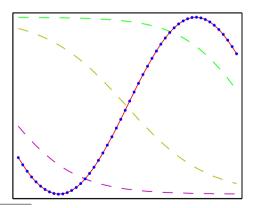


From Bishop's Pattern Recognition and Machine Learning, Fig 5.3

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Approximation Ability: $f(x) = \sin(x)$

- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.

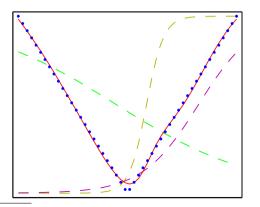


From Bishop's Pattern Recognition and Machine Learning, Fig 5.3

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Approximation Ability: f(x) = |x|

- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.

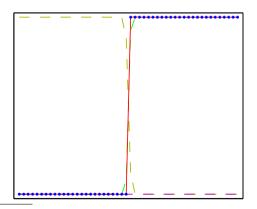


From Bishop's Pattern Recognition and Machine Learning, Fig 5.3

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Approximation Ability: f(x) = 1(x > 0)

- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



From Bishop's Pattern Recognition and Machine Learning, Fig 5.3

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Universal approximation theorems

How much expressive power do we gain from the nonlinearity?

Theorem (Universal approximation theorem)

A neural network with one possibly huge hidden layer $\hat{F}(x)$ can approximate any continuous function F(x) on a closed and bounded subset of \mathbb{R}^d under mild assumptions on the activation function, i.e. $\forall \epsilon > 0$, there exists an integer N s.t.

$$\hat{F}(x) = \sum_{i=1}^{N} w_i \sigma(v_i^T x + b_i)$$
(7)

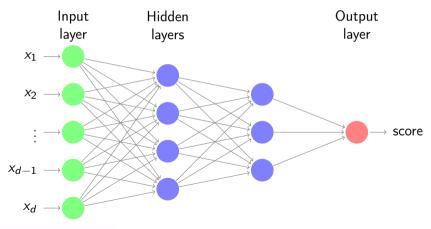
satisfies $|\hat{F}(x) - F(x)| < \epsilon$.

- Number of hidden units needs to be exponential in d.
- Doesn't say how to learn these parameters.

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Multilayer perceptron / Feed-forward neural networks

- Wider: more hidden units.
- Deeper: more hidden layers.



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Multilayer Perceptron: Standard Recipe

- Input space: $X = \mathbb{R}^d$ Action space $A = \mathbb{R}^k$ (for k-class classification).
- Let $\sigma: R \to R$ be an activation function (e.g. tanh or ReLU).
- Let's consider an MLP of L hidden layers, each having m hidden units.
- First hidden layer is given by

$$h^{(1)}(x) = \sigma\left(W^{(1)}x + b^{(1)}\right),$$

for parameters $W^{(1)} \in \mathbb{R}^{m \times d}$ and $b \in \mathbb{R}^m$, and where $\sigma(\cdot)$ is applied to each entry of its argument.

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Multilayer Perceptron: Standard Recipe

• Each subsequent hidden layer takes the output $o \in \mathbb{R}^m$ of previous layer and produces

$$h^{(j)}(o^{(j-1)}) = \sigma(W^{(j)}o^{(j-1)} + b^{(j)}), \text{ for } j = 2, ..., L$$

where $W^{(j)} \in \mathbb{R}^{m \times m}$, $b^{(j)} \in \mathbb{R}^m$.

• Last layer is an affine mapping (no activation function):

$$a(o^{(L)}) = W^{(L+1)}o^{(L)} + b^{(L+1)},$$

where $W^{(L+1)} \in \mathbb{R}^{k \times m}$ and $b^{(L+1)} \in \mathbb{R}^k$.

• The full neural network function is given by the *composition* of layers:

$$f(x) = \left(a \circ h^{(L)} \circ \dots \circ h^{(1)}\right)(x) \tag{8}$$

• Last layer typically gives us a score. How to do classification?

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Multinomial Logistic Regression

• From each x, we compute a linear score function for each class:

$$x \mapsto (\langle w_1, x \rangle, \dots, \langle w_k, x \rangle) \in \mathbb{R}^k$$

- We need to map this R^k vector into a probability vector θ .
- The softmax function maps scores $s = (s_1, ..., s_k) \in \mathbb{R}^k$ to a categorical distribution:

$$(s_1, \dots, s_k) \mapsto \theta = \operatorname{Softmax}(s_1, \dots, s_k) = \left(\frac{\exp(s_1)}{\sum_{i=1}^k \exp(s_i)}, \dots, \frac{\exp(s_k)}{\sum_{i=1}^k \exp(s_i)}\right)$$

$$\operatorname{P(y=1)}(s_1, \dots, s_k) \mapsto \theta = \operatorname{Softmax}(s_1, \dots, s_k) = \left(\frac{\exp(s_1)}{\sum_{i=1}^k \exp(s_i)}, \dots, \frac{\exp(s_k)}{\sum_{i=1}^k \exp(s_i)}\right)$$

Nonlinear Generalization of Multinomial Logistic Regression

• From each x, we compute a non-linear score function for each class:

$$x \mapsto (f_1(x), \dots, f_k(x)) \in \mathbb{R}^k$$

where f_i 's are outputs of the last hidden layer of a neural network.

• Learning: Maximize the log-likelihood of training data

$$\underset{f_1,\ldots,f_k}{\operatorname{arg\,max}} \sum_{i=1}^n \log \left[\operatorname{Softmax} \left(f_1(x),\ldots,f_k(x) \right)_{y_i} \right].$$

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Neural network as a feature extractor

- OverFeat is a neural network for object classification, localization, and detection.
 - Trained on the huge ImageNet dataset
 - Lots of computing resources used for training the network.
- All those hidden layers of the network are very valuable features.
 - Paper: "CNN Features off-the-shelf: an Astounding Baseline for Recognition"
 - Showed that using features from OverFeat makes it easy to achieve state-of-the-art performance on new vision tasks.

We've seen

- Key idea: automatically discover useful features from raw data—feature/representation learning.
- Building blocks:

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Input layer no learnable parameters

Hidden layer(s) perceptron + nonlinear activation function

Output layer affine (+ transformation)
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- A single hidden layer is sufficient to approximate any function.
- In practice, often have multiple hidden layers.

Next, how to learn the parameters.

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