Feature Learning

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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:

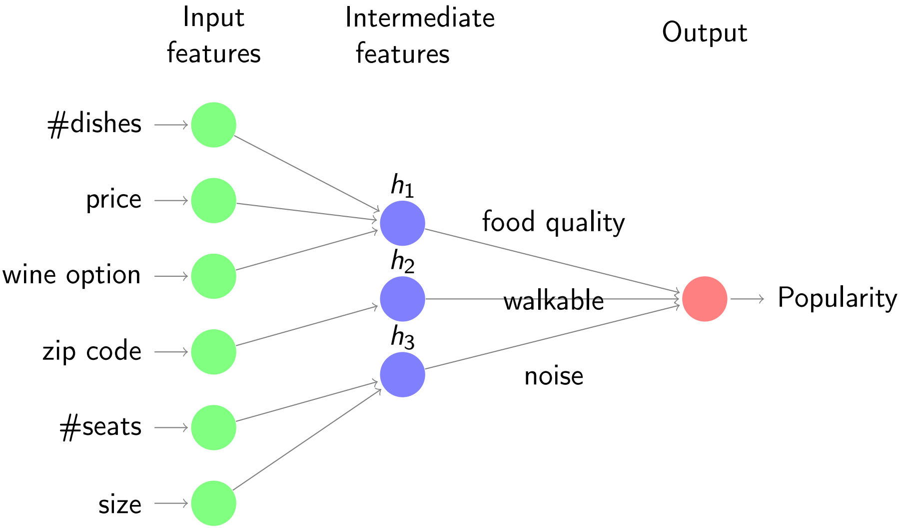
  Task: Predict popularity of restaurants.

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

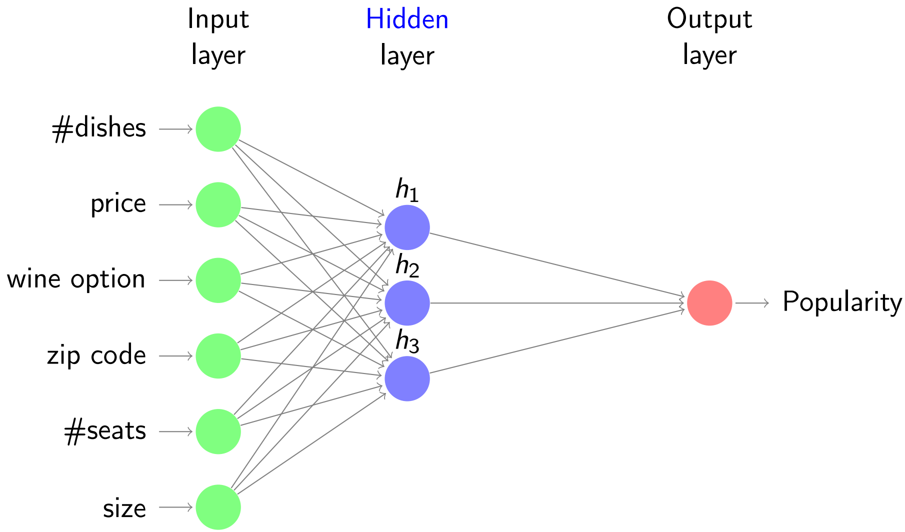
- Decompose into subproblems:
  - $h_1([\#\text{dishes, price, wine option}]) = \text{food quality}$
  - $h_2([\text{zip code}]) = \text{walkable}$
  - $h_3([\#\text{seats, size}]) = \text{nosie}$
- Final *linear* predictor uses **intermediate features** computed by h_i's:

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

Predefined subproblems



Learned intermediate features



Key idea: automatically learn the intermediate features.

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

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

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

$$h(x) = [h_1(x), \ldots, h_K(x)], \tag{3}$$

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

Activation function

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

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

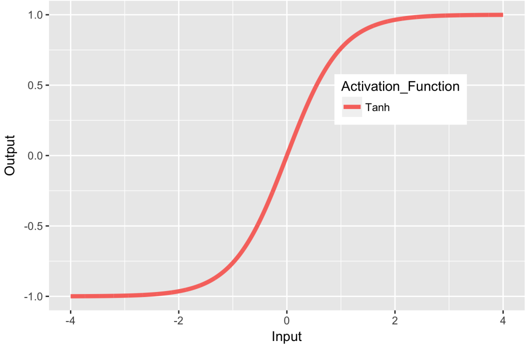
- σ is the *nonlinear* **activation function**.
- What might be some activation functions we want to use?
  - sign function? Non-differentiable.
  - *Differentiable* approximations: sigmoid functions.
    - E.g., logistic function, hyperbolic tangent function.
- Two-layer neural network (one hidden layer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

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

Activation Functions

- The **hyperbolic tangent** is a common activation function:

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

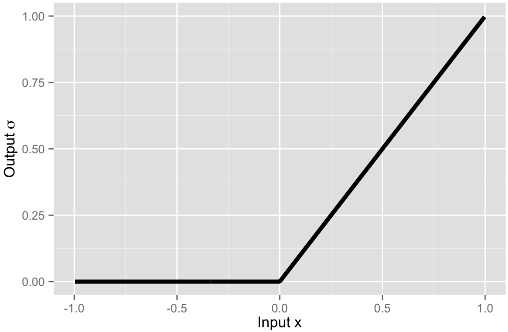


Activation Functions

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

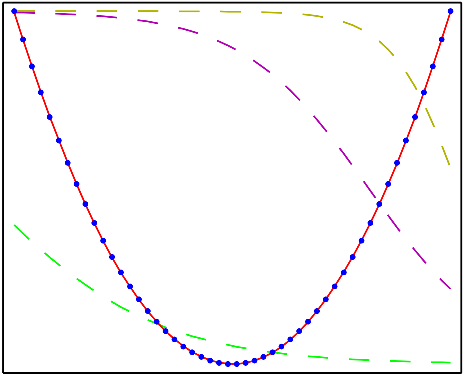
$$\sigma(x) = \max(0, x).$$

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



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

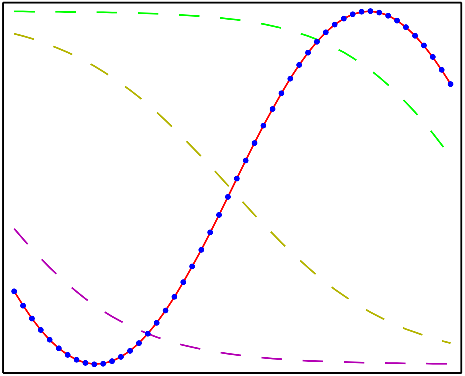
- 3 hidden units; tanh activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

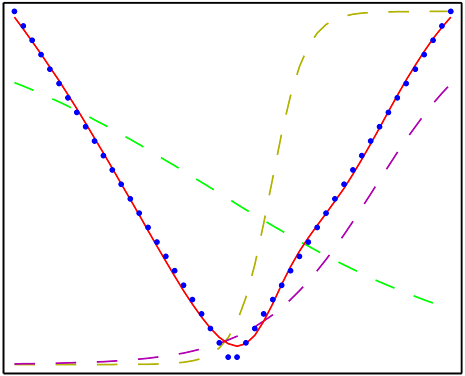
- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

Approximation Ability: $f(x) = |x|$

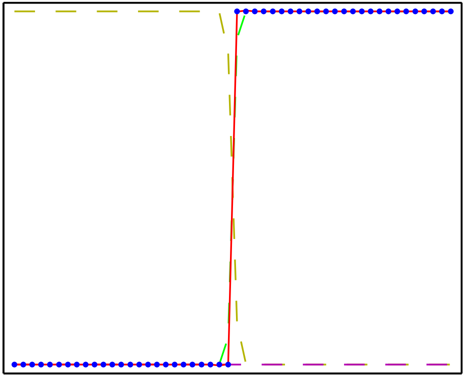
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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.



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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.

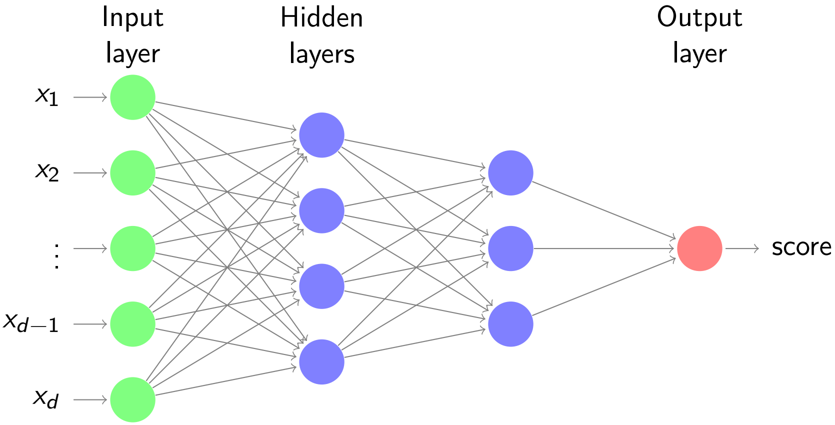
$$\hat{F}(x) = \sum_{i=1}^{N} w_i \sigma(v_i^T x + b_i) \tag{7}$$

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.

Multilayer perceptron / Feed-forward neural networks

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



- **Input space**: $\mathcal{X} = \mathbb{R}^d$ **Action space** $\mathcal{A} = \mathbb{R}^k$ (for k-class classification).
- Let $\sigma : \mathbb{R} \to \mathbb{R}$ 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.

Multilayer Perceptron: Standard Recipe

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

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

  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:

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

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

Multinomial Logistic Regression

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

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

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

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

Nonlinear Generalization of Multinomial Logistic Regression

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

$$x \mapsto (f_1(x), \ldots, f_k(x)) \in \mathrm{R}^k$$

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

- Learning: Maximize the log-likelihood of training data

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

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.

OverFeat code is at https://github.com/sermanet/OverFeat

Review

We've seen

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

Input layer	no learnable parameters
Hidden layer(s)	perceptron + *nonlinear* activation function
Output layer	affine (+ transformation)

- A single hidden layer is sufficient to approximate any function.
- In practice, often have multiple hidden layers.

Next, how to learn the parameters.