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Connecting Machine Learning with Shallow Neural Networks

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.1

Neural Networks and Machine Learning

- Neural networks are optimization-based learning models.

- Many classical machine learning models use continuous optimization:

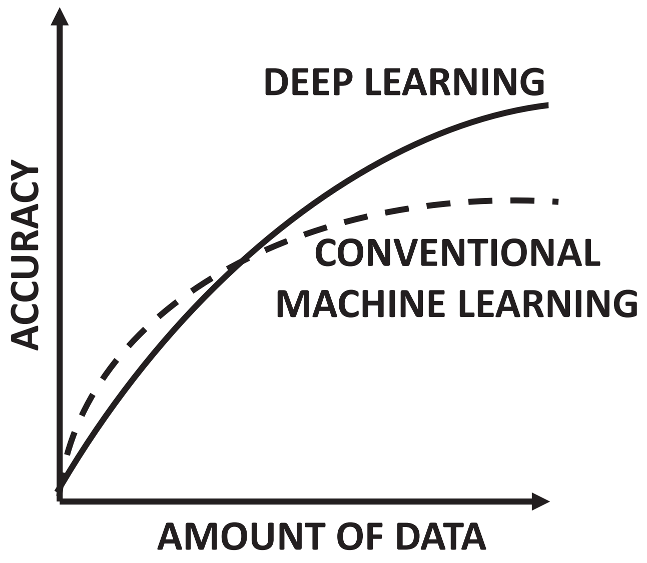
  - SVMs, Linear Regression, and Logistic Regression

  - Singular Value Decomposition

  - (Incomplete) Matrix factorization for Recommender Systems

- All these models can be represented as special cases of shallow neural networks!

The Continuum Between Machine Learning and Deep Learning



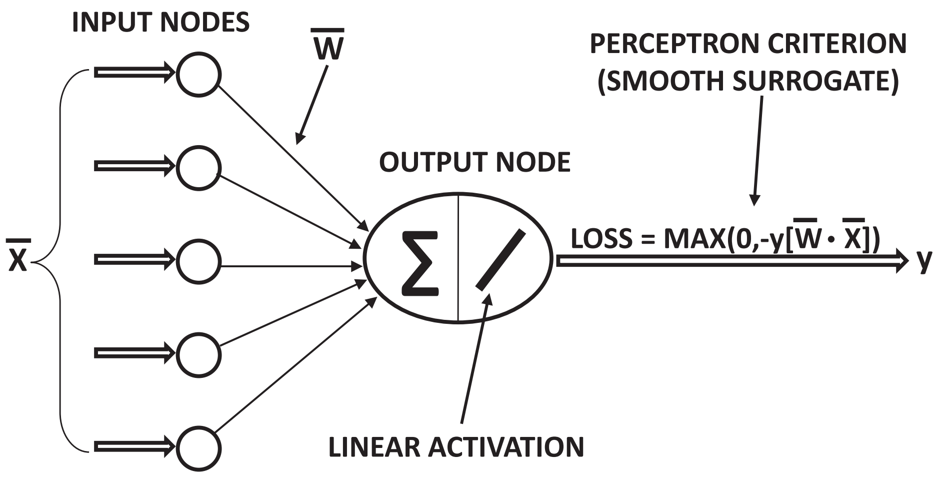
- Classical machine learning models reach their learning capacity early because they are simple neural networks.

- When we have more data, we can add more computational units to improve performance.

The Deep Learning Advantage

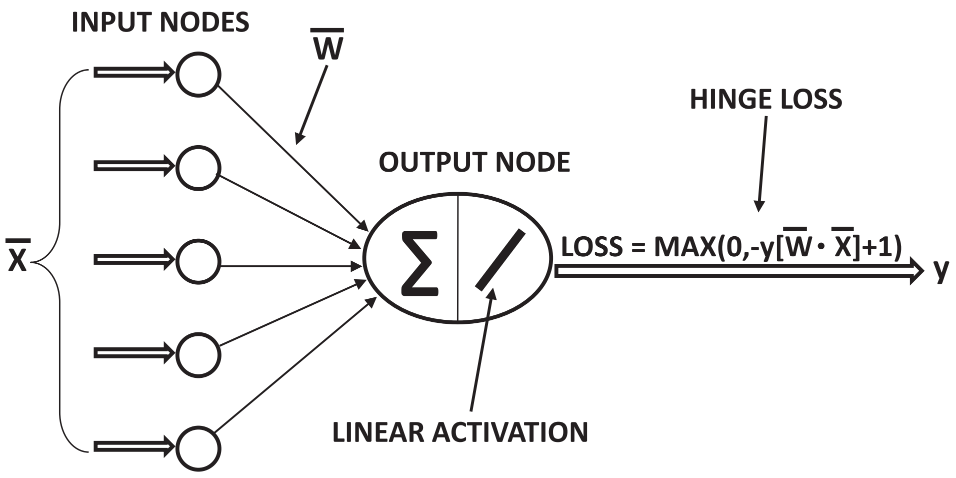
- Exploring the neural models for traditional machine learning is useful because it exposes the cases in which deep learning has an advantage.
  - Add capacity with more nodes for more data.
  - Controlling the structure of the architecture provides a way to incorporate domain-specific insights (e.g., recurrent networks and convolutional networks).
- In some cases, making minor changes to the architecture leads to interesting models:
  - Adding a sigmoid/softmax layer in the output of a neural model for (linear) matrix factorization can result in logistic/multinomial matrix factorization (e.g., word2vec).

Recap: Perceptron versus Linear Support Vector Machine



(a) Perceptron

Loss $= \max\{0, -y(\overline{W} \cdot \overline{X})\}$



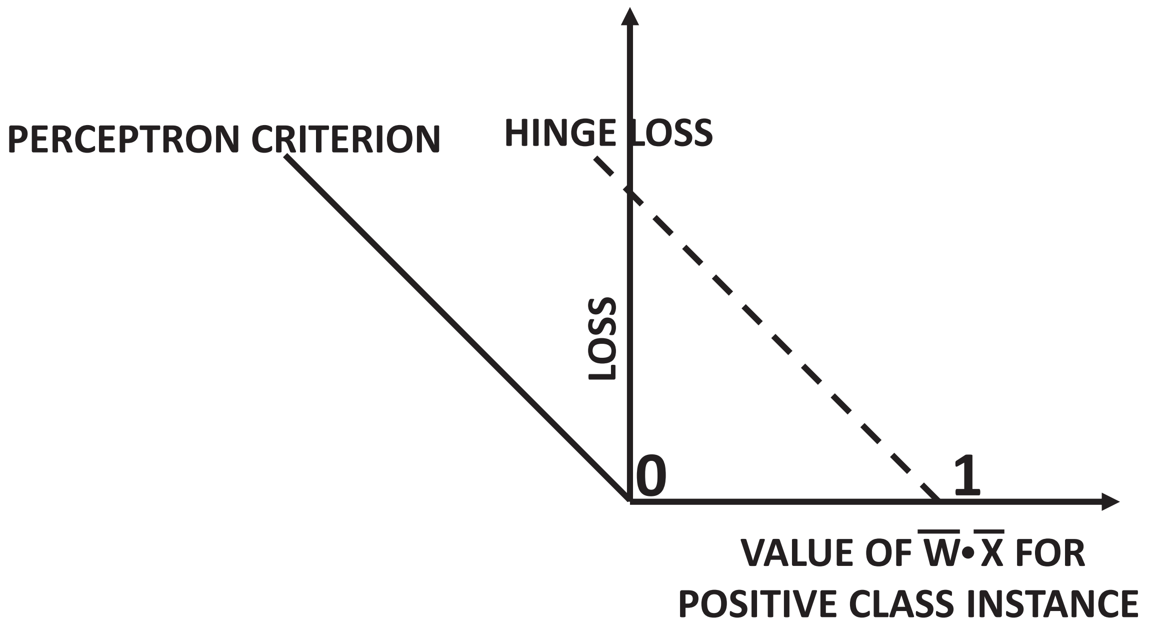
(b) SVM

Loss $= \max\{0, 1 - y(\overline{W} \cdot \overline{X})\}$

- The Perceptron criterion is a minor variation of hinge loss with identical update of $\overline{W} \Leftarrow \overline{W} + \alpha y \overline{X}$ in both cases.

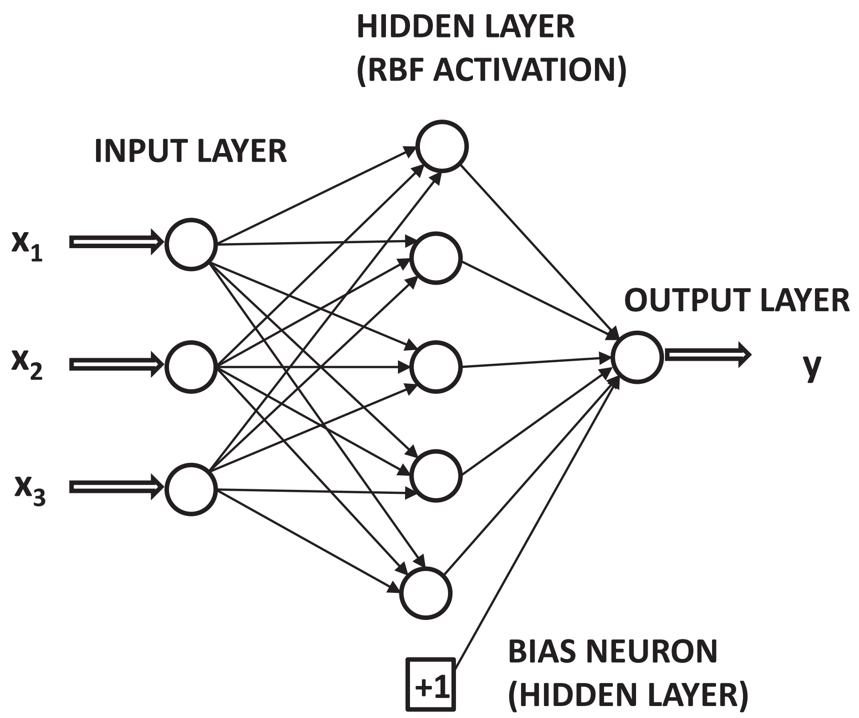
- We update only for misclassified instances in perceptron, but update *also* for "marginally correct" instances in SVM.

Perceptron Criterion versus Hinge Loss



- Loss for positive class training instance at varying values of $\overline{W} \cdot \overline{X}$.

What About the Kernel SVM?



- RBF Network for unsupervised feature engineering.
  - Unsupervised feature engineering is good for noisy data.
  - Supervised feature engineering (with deep learning) is good for learning rich structure.

Much of Machine Learning is a Shallow Neural Model

- By minor changes to the architecture of perceptron we can get:
  - Linear regression, Fisher discriminant, and Widrow-Hoff learning $\Rightarrow$ Linear activation in output node
  - Logistic regression $\Rightarrow$ Sigmoid activation in output node
- Multinomial logistic regression $\Rightarrow$ Softmax Activation in Final Layer
- Singular value decomposition $\Rightarrow$ Linear autoencoder
- Incomplete matrix factorization for Recommender Systems $\Rightarrow$ Autoencoder-like architecture with single hidden layer (also used in *word2vec*)

Why do We Care about Connections?

- Connections tell us about the cases that it makes sense to use conventional machine learning:
  - If you have less data with noise, you want to use conventional machine learning.
  - If you have a lot of data with rich structure, you want to use neural networks.
  - Structure is often learned by using deep neural architectures.
- Architectures like convolutional neural networks can use domain-specific insights.

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Neural Models for Linear Regression, Classification, and the Fisher Discriminant [Connections with Widrow-Hoff Learning]

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.2

Widrow-Hoff Rule: The Neural Avatar of Linear Regression

- The perceptron (1958) was historically followed by Widrow-Hoff Learning (1960).

- Identical to linear regression when applied to numerical targets.

  - Originally proposed by Widrow and Hoff for binary targets (not natural for regression).

- The Widrow-Hoff method, when applied to mean-centered features and mean-centered binary class encoding, learns the Fisher discriminant.

- We first discuss linear regression for numeric classes and then visit the case of binary classes.

Linear Regression: An Introduction

- In linear regression, we have training pairs $(\overline{X}_i, y_i)$ for $i \in \{1 \ldots n\}$, so that $\overline{X_i}$ contains d-dimensional features and y_i contains a numerical target.

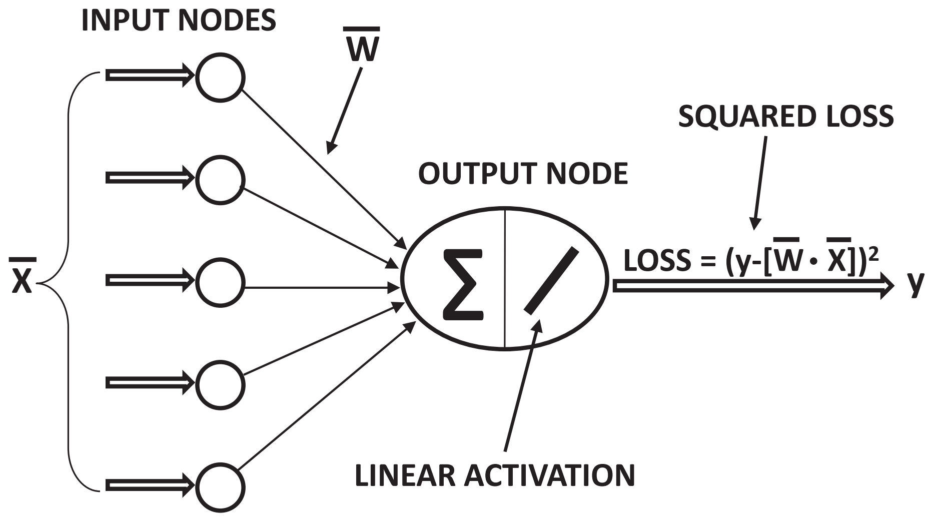
- We use a linear parameterized function to predict $\hat{y}_i = \overline{W} \cdot \overline{X}_i$.

- Goal is to learn $\overline{W}$, so that the sum-of-squared differences between observed y_i and predicted $\hat{y}_i$ is minimized over the entire training data.

- Solution exists in closed form, but requires the inversion of a potentially large matrix.

- Gradient-descent is typically used anyway.

Linear Regression with Numerical Targets:Neural Model



- Predicted output is $\hat{y}_i = \overline{W} \cdot \overline{X}_i$ and loss is $L_i = (y_i - \hat{y}_i)^2$.

- Gradient-descent update is $\overline{W} \Leftarrow \overline{W} - \alpha \frac{\partial L_i}{\partial \overline{W}} = \overline{W} + \alpha (y_i - \hat{y}_i) \overline{X}_i$.

Widrow-Hoff: Linear Regression with Binary Targets

- For $y_i \in \{-1, +1\}$, we use same loss of $(y_i - \widehat{y}_i)^2$, and update of $\overline{W} \Leftarrow \overline{W} + \alpha \underbrace{(y_i - \widehat{y}_i)}_{\text{delta}} \overline{X}_i$.
  - When applied to binary targets, it is referred to as delta rule.
  - Perceptron uses the same update with $\widehat{y}_i = \text{sign}\{\overline{W} \cdot \overline{X}_i\}$, whereas Widrow-Hoff uses $\widehat{y}_i = \overline{W} \cdot \overline{X}_i$.

- **Potential drawback:** Retrogressive treatment of well-separated points caused by the pretension that binary targets are real-valued.
  - If $y_i = +1$, and $\overline{W} \cdot \overline{X}_i = 10^6$, the point will be heavily penalized for strongly correct classification!
  - Does not happen in perceptron.

Comparison of Widrow-Hoff with Perceptron and SVM

- Convert the binary loss functions and updates to a form more easily comparable to perceptron using $y_i^2 = 1$:

- Loss of $(\overline{X}_i, y_i)$ is $(y_i - \overline{W} \cdot \overline{X}_i)^2 = (1 - y_i[\overline{W} \cdot \overline{X}_i])^2$
  Update: $\overline{W} \Leftarrow \overline{W} + \alpha y_i (1 - y_i[\overline{W} \cdot \overline{X}_i])\overline{X}_i$

	Perceptron	L_1-Loss SVM
Loss	$\max\{-y_i(\overline{W} \cdot \overline{X}_i), 0\}$	$\max\{1 - y_i(\overline{W} \cdot \overline{X}_i), 0\}$
Update	$\overline{W} \Leftarrow \overline{W} + \alpha y_i I(-y_i[\overline{W} \cdot \overline{X}_i] > 0)\overline{X}_i$	$\overline{W} \Leftarrow \overline{W} + \alpha y_i I(1 - y_i[\overline{W} \cdot \overline{X}_i] > 0)\overline{X}_i$

	Widrow-Hoff	Hinton's L_2-Loss SVM
Loss	$(1 - y_i(\overline{W} \cdot \overline{X}_i))^2$	$\max\{1 - y_i(\overline{W} \cdot \overline{X}_i), 0\}^2$
Update	$\overline{W} \Leftarrow \overline{W} + \alpha y_i (1 - y_i[\overline{W} \cdot \overline{X}_i])\overline{X}_i$	$\overline{W} \Leftarrow \overline{W} + \alpha y_i \max\{(1 - y_i[\overline{W} \cdot \overline{X}_i]), 0\}\overline{X}_i$

Some Interesting Historical Facts

- Hinton proposed the SVM L_2-loss three years before Cortes and Vapnik's paper on SVMs.
  - G. Hinton. Connectionist learning procedures. *Artificial Intelligence*, 40(1–3), pp. 185–234, 1989.
  - Hinton's L_2-loss was proposed to address some of the weaknesses of loss functions like linear regression on binary targets.
  - When used with L_2-regularization, it behaves identically to an L_2-SVM, but the connection with SVM was overlooked.
- The Widrow-Hoff rule is also referred to as ADALINE, LMS (least mean-square method), delta rule, and least-squares classification.

Connections with Fisher Discriminant

- Consider a binary classification problem with training instances $(\overline{X}_i, y_i)$ and $y_i \in \{-1, +1\}$.
  - Mean-center each feature vector as $\overline{X}_i - \overline{\mu}$.
  - Mean-center the binary class by subtracting $\sum_{i=1}^{n} y_i/n$ from each y_i.
- Use the delta rule $\overline{W} \Leftarrow \overline{W} + \alpha \underbrace{(y_i - \hat{y}_i)}_{\text{delta}} \overline{X}_i$ for learning.
- Learned vector is the Fisher discriminant!
  - Proof in Christopher Bishop's book on machine learning.

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Neural Models for Logistic Regression

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.2

Logistic Regression: A Probabilistic Model

- Consider the training pair $(\overline{X}_i, y_i)$ with d-dimensional feature variables in $\overline{X_i}$ and class variable $y_i \in \{-1, +1\}$.

- In logistic regression, the sigmoid function is applied to $\overline{W} \cdot \overline{X}_i$, which predicts the probability that y_i is $+1$.

$$\hat{y}_i = P(y_i = 1) = \frac{1}{1 + \exp(-\overline{W} \cdot \overline{X}_i)}$$

- We want to *maximize* $\hat{y}_i$ for positive class instances and $1 - \hat{y}_i$ for negative class instances.

  – Same as *minimizing* $-\log(\hat{y}_i)$ for positive class instances and $-\log(1 - \hat{y}_i)$ for negative instances.

  – Same as minimizing loss $L_i = -\log(|y_i/2 - 0.5 + \hat{y}_i|)$.

  – Alternative form of loss $L_i = \log(1 + \exp[-y_i(\overline{W} \cdot \overline{X}_i)])$

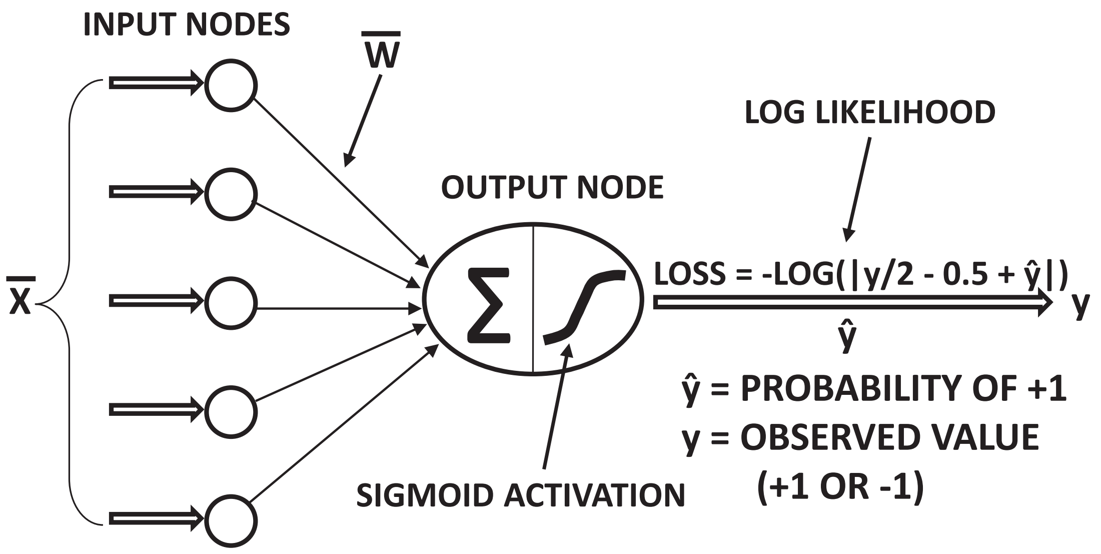
Maximum-Likelihood Objective Functions

- Why did we use the negative logarithms?

- Logistic regression is an example of a maximum-likelihood objective function.

- Our goal is to maximize the *product* of the probabilities of correct classification over all training instances.
  - Same as minimizing the *sum* of the negative log probabilities.
  - Loss functions are always *additive* over training instances.
  - So we are really minimizing $\sum_i -\log(|y_i/2 - 0.5 + \hat{y}_i|)$ which can be shown to be $\sum_i \log(1 + \exp[-y_i(\overline{W} \cdot \overline{X}_i)])$.

Logistic Regression: Neural Model



- Predicted output is $\hat{y}_i = 1/(1 + \exp(-\overline{W} \cdot \overline{X}_i))$ and loss is $L_i = -\log(|y_i/2 - 0.5 + \hat{y}_i|) = \log(1 + \exp[-y_i(\overline{W} \cdot \overline{X}_i)])$.
  - Gradient-descent update is $\overline{W} \Leftarrow \overline{W} - \alpha \frac{\partial L_i}{\partial \overline{W}}$.

$$\overline{W} \Leftarrow \overline{W} + \alpha \frac{y_i \overline{X_i}}{1 + \exp[y_i(\overline{W} \cdot \overline{X_i})]}$$

Interpreting the Logistic Update

- An important multiplicative factor in the update increment is $1/(1+\exp[y_i(\overline{W} \cdot \overline{X}_i)])$.

- This factor is $1-\hat{y}_i$ for positive instances and $\hat{y}_i$ for negative instances $\Rightarrow$ Probability of mistake!

- Interpret as: $\overline{W} \Leftarrow \overline{W} + \alpha \left[\text{Probability of mistake on } (\overline{X_i}, y_i)\right] (y_i \overline{X_i})$

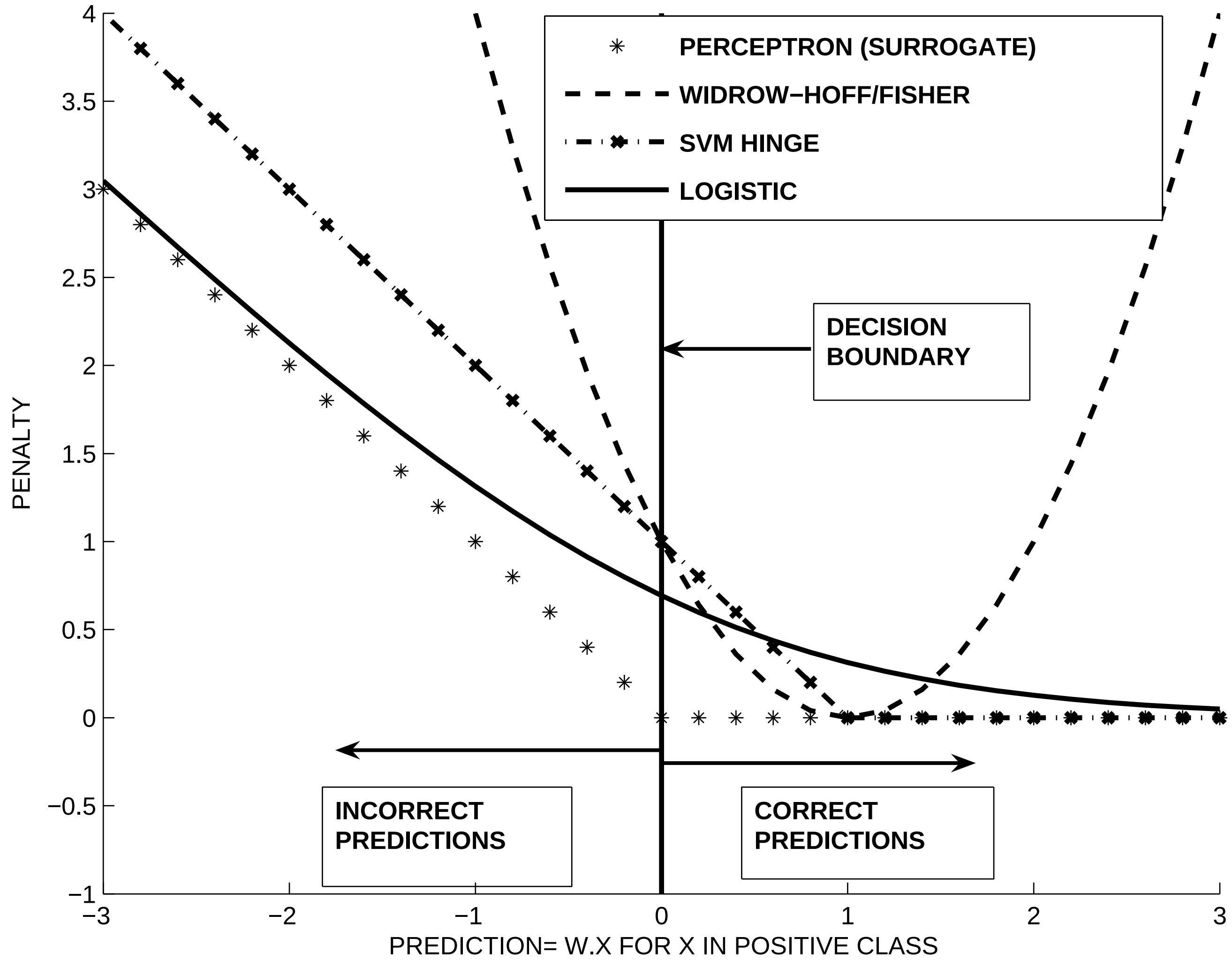
Comparing Updates of Different Models

- The unregularized updates of the perceptron, SVM, Widrow-Hoff, and logistic regression can all be written in the following form:

$$\overline{W} \Leftarrow \overline{W} + \alpha y_i \delta(\overline{X}_i, y_i)\overline{X}_i$$

- The quantity $\delta(\overline{X}_i, y_i)$ is a *mistake function*, which is:
  - Raw mistake value $(1 - y_i(\overline{W} \cdot \overline{X}_i))$ for Widrow-Hoff
  - Mistake indicator whether $(0 - y_i(\overline{W} \cdot \overline{X}_i)) > 0$ for perceptron.
  - Margin/mistake indicator whether $(1 - y_i(\overline{W} \cdot \overline{X}_i)) > 0$ for SVM.
  - Probability of mistake on $(\overline{X}_i, y_i)$ for logistic regression.

Comparing Loss Functions of Different Models



- Loss functions are similar (note Widrow-Hoff retrogression).

Other Comments on Logistic Regression

- Many classical neural models use repeated computational units with logistic and tanh activation functions in hidden layers.

- One can view these methods as feature engineering models that stack multiple logistic regression models.

- The stacking of multiple models creates inherently more powerful models than their individual components.

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The Softmax Activation Function and Multinomial Logistic Regression

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.3

Binary Classes versus Multiple Classes

- All the models discussed so far discuss only the binary class setting in which the class label is drawn from $\{-1, +1\}$.

- Many natural applications contain multiple classes without a natural ordering among them:
  - Predicting the category of an image (e.g., *truck*, *carrot*).
  - *Language models:* Predict the next word in a sentence.

- Models like logistic regression are naturally designed to predict two classes.

Generalizing Logistic Regression

- Logistic regression produces probabilities of the two outcomes of a binary class.

- *Multinomial* logistic regression produces probabilities of multiple outcomes.

  - In order to produce probabilities of multiple classes, we need an activation function with a vector output of probabilities.

  - The *softmax activation function* is a vector-based generalization of the sigmoid activation used in logistic regression.

- Multinomial logistic regression is also referred to as softmax classifier.

The Softmax Activation Function

- The softmax activation function is a natural vector-centric generalization of the scalar-to-scalar sigmoid activation $\Rightarrow$ vector-to-vector function.

- Logistic sigmoid activation: $\Phi(v) = 1/(1 + \text{exp}(-v))$.

- Softmax activation: $\Phi(v_1 \ldots v_k) = \frac{1}{\sum_{i=1}^{k} \text{exp}(v_i)} [\text{exp}(v_1) \ldots \text{exp}(v_k)]$

  – The k outputs (probabilities) sum to 1.

- Binary case of using sigmoid(v) is identical to using 2-element softmax activation with arguments $(v, 0)$.

  – Multinomial logistic regression with 2-element softmax is equivalent to binary logistic regression.

Loss Functions for Softmax

- Recall that we use the negative logarithm of the probability of observed class in binary logistic regression.
  - Natural generalization to multiple classes.
  - Cross-entropy loss: Negative logarithm of the probability of correct class.
  - Probability distribution among incorrect classes has no effect.
- Softmax activation is used almost exclusively in output layer and (almost) always paired with cross-entropy loss.

Cross-Entropy Loss of Softmax

- Like the binary logistic case, the loss L is a negative log probability.

$$\text{Softmax Probability Vector} \Rightarrow [\widehat{y}_1, \widehat{y}_2, \ldots \widehat{y}_k]$$

$$[\widehat{y}_1 \ldots \widehat{y}_k] = \frac{1}{\sum_{i=1}^{k} \exp(v_i)} [\exp(v_1) \ldots \exp(v_k)]$$

- The loss is $-\log(\widehat{y}_c)$, where $c \in \{1 \ldots k\}$ is the correct class of that training instance.

- Cross entropy loss is $-v_{c)} + \log[\sum_{j=1}^{k} \exp(v_j)]$

Loss Derivative of Softmax

- Since softmax is almost always paired with cross-entropy loss L, we can directly estimate $\frac{\partial L}{\partial v_r}$ for each pre-activation value from $v_1 \ldots v_k$.

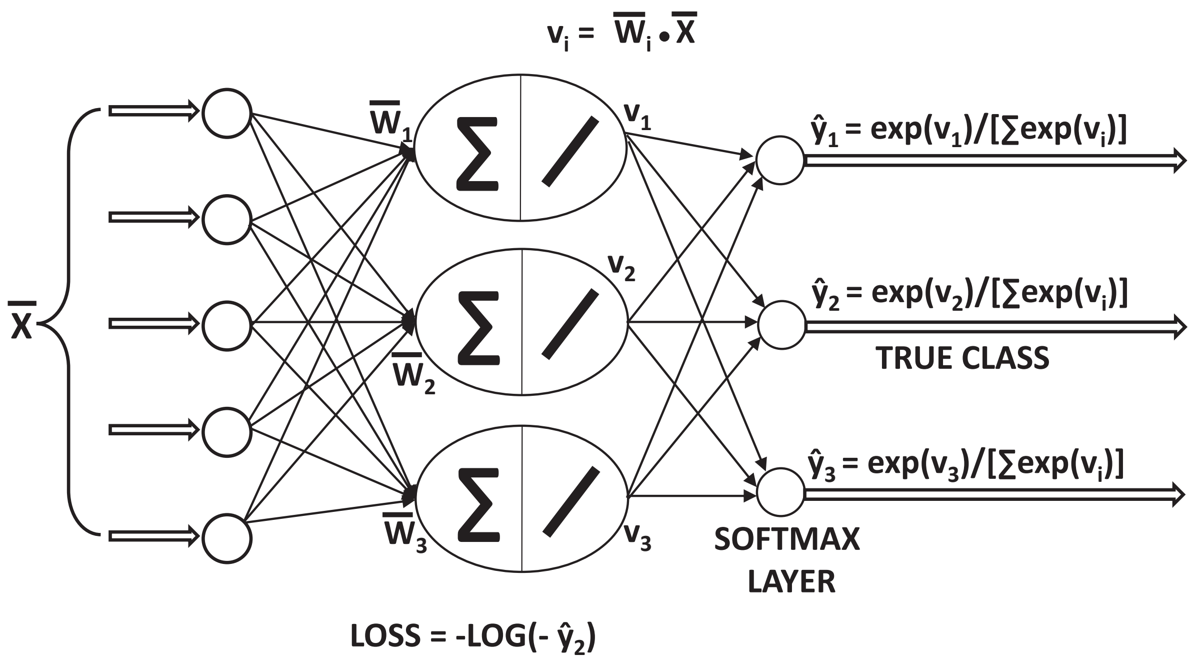
- Differentiate loss value of $-v_c + \log[\sum_{j=1}^{k} \exp(v_j)]$

- Like the sigmoid derivative, the result is best expressed in terms of the post-activation values $\widehat{y}_1 \ldots \widehat{y}_k$.

- The loss derivative of the softmax is as follows:

$$\frac{\partial L}{\partial v_r} = \begin{cases} \widehat{y}_r - 1 & \text{If } r \text{ is correct class} \\ \widehat{y}_r & \text{If } r \text{ is not correct class} \end{cases}$$

Multinomial Logistic Regression



- The ith training instance is $(\overline{X_i}, c(i))$, where $c(i) \in \{1 \ldots k\}$ is class index $\Rightarrow$ Learn k parameter vectors $\overline{W}_1 \ldots \overline{W}_k$.
  - Define real-valued score $v_r = \overline{W}_r \cdot \overline{X}_i$ for rth class.
  - Convert scores to probabilities $\hat{y}_1 \ldots \hat{y}_k$ with softmax activation on $v_1 \ldots v_k$ $\Rightarrow$ Hard or soft prediction

Computing the Derivative of the Loss

- The cross-entropy loss for the ith training instance is $L_i = -\log(\widehat{y}_{c(i)})$.

- For gradient-descent, we need to compute $\frac{\partial L_i}{\partial \overline{\overline{W}}_r}$.

- Using chain rule of differential calculus, we get:

$$\frac{\partial L_i}{\partial \overline{\overline{W}}_r} = \sum_j \left(\frac{\partial L_i}{\partial v_j}\right)\left(\frac{\partial v_j}{\partial \overline{\overline{W}}_r}\right) = \frac{\partial L_i}{\partial v_r} \underbrace{\frac{\partial v_r}{\partial \overline{\overline{W}}_r}}_{\overline{X_i}} + \text{Zero-terms}$$

$$= \begin{cases} -\overline{X_i}(1-\widehat{y}_r) & \text{if } r = c(i) \\ \overline{X_i}\,\widehat{y}_r & \text{if } r \neq c(i) \end{cases}$$

Gradient Descent Update

- Each separator $\overline{W_r}$ is updated using the gradient:

$$\overline{W_r} \Leftarrow \overline{W_r} - \alpha \frac{\partial L_i}{\partial \overline{W_r}}$$

- Substituting the gradient from the previous slide, we obtain:

$$\overline{W_r} \Leftarrow \overline{W_r} + \alpha \begin{cases} \overline{X_i} \cdot (1 - \widehat{y}_r) & \text{if } r = c(i) \\ -\overline{X_i} \cdot \widehat{y}_r & \text{if } r \neq c(i) \end{cases}$$

Summary

- The book also contains details of the multiclass Perceptron and Weston-Watkins SVM.

- Multinomial logistic regression is a direct generalization of logistic regression.

- If we apply the softmax classifier with two classes, we will obtain $\overline{W_1} = -\overline{W_2}$ to be the same separator as obtained in logistic regression.

- Cross-entropy loss and softmax are almost always paired in output layer (for all types of architectures).

  – Many of the calculus derivations in previous slides are repeatedly used in different settings.

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The Autoencoder for Unsupervised Representation Learning

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.5

Unsupervised Learning

- The models we have discussed so far use training pairs of the form $(\overline{X}, y)$ in which the feature variables $\overline{X}$ and target y are clearly separated.
  - The target variable y provides the *supervision* for the learning process.
- What happens when we do not have a target variable?
  - We want to capture a model of the training data without the guidance of the target.
  - This is an *unsupervised* learning problem.

Example

- Consider a 2-dimensional data set in which all points are distributed on the circumference of an origin-centered circle.

- All points in the first and third quadrant belong to class $+1$ and remaining points are -1.

  – The class variable provides focus to the learning process of the supervised model.

  – An unsupervised model needs to recognize the circular manifold without being told up front.

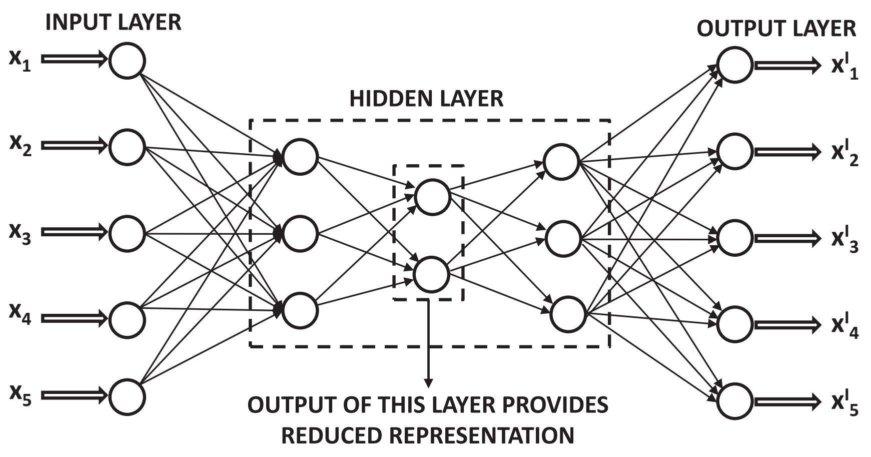
  – The unsupervised model can represent the data in only 1 dimension (angular position).

- Best way of modeling is data-set dependent $\Rightarrow$ Lack of supervision causes problems

Unsupervised Models and Compression

- Unsupervised models are closely related to compression because compression captures a model of regularities in the data.
  - Generative models represent the data in terms of a compressed parameter set.
  - Clustering models represent the data in terms of cluster statistics.
  - Matrix factorization represents data in terms of low-rank approximations (compressed matrices).
- An autoencoder also provides a compressed representation of the data.

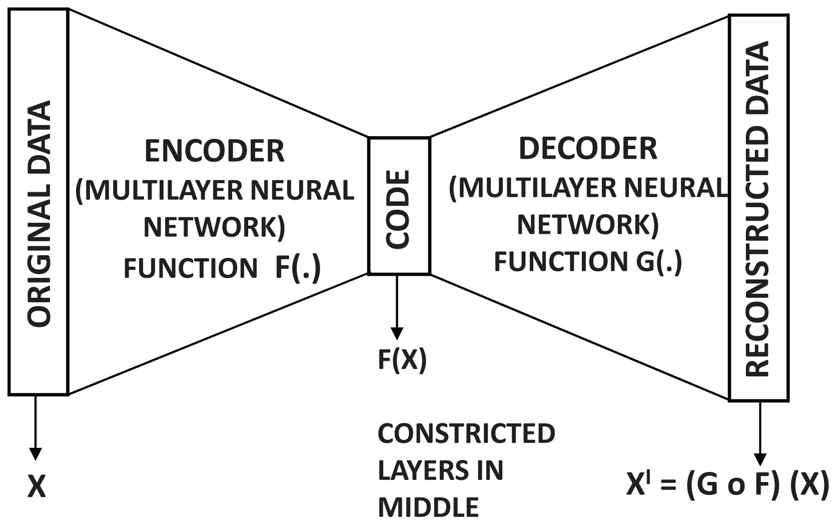
Defining the Input and Output of an Autoencoder



- All neural networks work with input-output pairs.
  - In a supervised problem, the output is the label.

- In the autoencoder, the output values are the same as inputs: *replicator neural network*.
  - The loss function penalizes a training instance depending on how far it is from the input (e.g., squared loss).

Encoder and Decoder



- Reconstructing the data might seem like a trivial matter by simply copying the data forward from one layer to another.
  - Not possible when the number of units in the middle are *constricted*.
  - Autoencoder is divided into *encoder* and *decoder*.

Basic Structure of Autoencoder

- It is common (but not necessary) for an M-layer autoencoder to have a symmetric architecture between the input and output.
  - The number of units in the kth layer is the same as that in the $(M - k + 1)$th layer.
- The value of M is often odd, as a result of which the $(M + 1)/2$th layer is often the most constricted layer.
  - We are counting the (non-computational) input layer as the first layer.
  - The minimum number of layers in an autoencoder would be three, corresponding to the input layer, constricted layer, and the output layer.

Undercomplete Autoencoders and Dimensionality Reduction

- The number of units in each middle layer is typically fewer than that in the input (or output).
  - These units hold a reduced representation of the data, and the final layer can no longer reconstruct the data exactly.
- This type of reconstruction is inherently *lossy*.
- The activations of hidden layers provide an alternative to linear and nonlinear dimensionality reduction techniques.

Overcomplete Autoencoders and Representation Learning

- What happens if the number of units in hidden layer is equal to or larger than input/output layers?
  - There are infinitely many hidden representations with zero error.
  - The middle layers often do not learn the identity function.
  - We can enforce specific properties on the redundant representations by adding constraints/regularization to hidden layer.
    - Training with stochastic gradient descent is itself a form of regularization.
    - One can learn sparse features by adding sparsity constraints to hidden layer.

Applications

- Dimensionality reduction $\Rightarrow$ Use activations of constricted hidden layer

- Sparse feature learning $\Rightarrow$ Use activations of constrained/regularized hidden layer

- Outlier detection: Find data points with larger reconstruction error
  - Related to denoising applications

- Generative models with probabilistic hidden layers (variational autoencoders)

- Representation learning $\Rightarrow$ Pretraining

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Singular Value Decomposition with Autoencoders

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.5

Singular Value Decomposition

- Truncated SVD is the *approximate* decomposition of an $n \times d$ matrix D into $D \approx Q\Sigma P^T$, where Q, Σ, and P are $n \times k$, $k \times k$, and $d \times k$ matrices, respectively.
  - Orthonormal columns of each of P, Q, and nonnegative diagonal matrix Σ.
  - Minimize the squared sum of residual entries in $D - Q\Sigma P^T$.
  - The value of k is typically much smaller than $\min\{n, d\}$.
  - Setting k to $\min\{n, d\}$ results in a zero-error decomposition.

Relaxed and Unnormalized Definition of SVD

- **Two-way Decomposition:** Find and $n \times k$ matrix U, and $d \times k$ matrix V so that $||D - UV^T||^2$ is minimized.
  - Property: At least one optimal pair U and V will have mutually orthogonal columns (but non-orthogonal alternatives will exist).
  - The orthogonal solution can be converted into the 3-way factorization of SVD.
  - Exercise: Given U and V with orthogonal columns, find Q, Σ and P.
- In the event that U and V have non-orthogonal columns at optimality, these columns will span the same subspace as the orthogonal solution at optimality.

Dimensionality Reduction and Matrix Factorization

- Singular value decomposition is a dimensionality reduction method (like any matrix factorization technique).

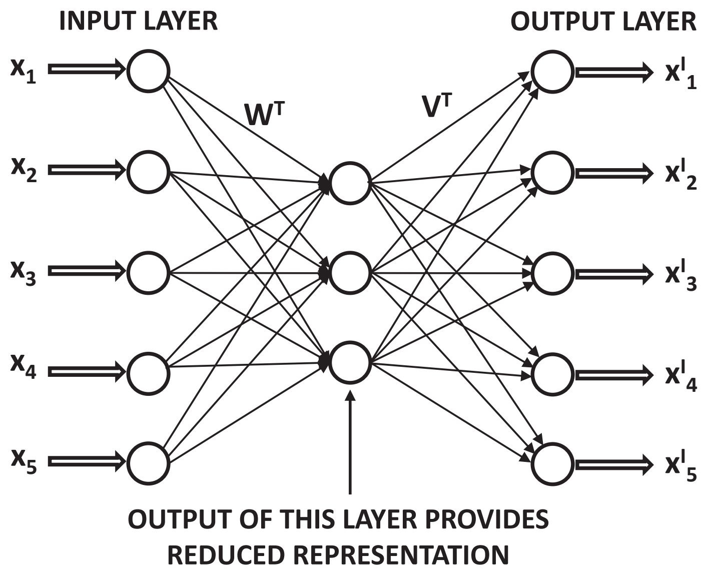
$$D \approx UV^T$$

- The n rows of D contain the n training points.

- The n rows of U provide the reduced representations of the training points.

- The k columns of V contain the orthogonal basis vectors.

The Autoencoder Architecture for SVD



- The rows of the matrix D are input to encoder.

- The activations of hidden layer are rows of U and the weights of the decoder contain V.

- The reconstructed data contain the rows of UV^T.

Why is this SVD?

- If we use the mean-squared error as the loss function, we are optimizing $||D - UV^T||^2$ over the entire training data.
  - This is the same objective function as SVD!

- It is possible for gradient-descent to arrive at an optimal solution in which the columns of each of U and V might not be mutually orthogonal.

- Nevertheless, the subspace spanned by the columns of each of U and V will always be the same as that found by the optimal solution of SVD.

Some Interesting Facts

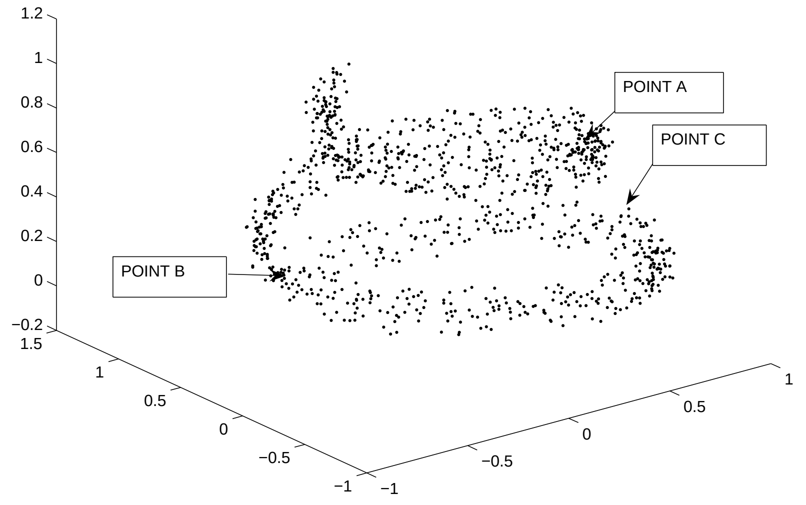
- The optimal encoder weight matrix W will be the pseudo-inverse of the decoder weight matrix V if the training data spans the full dimensionality.

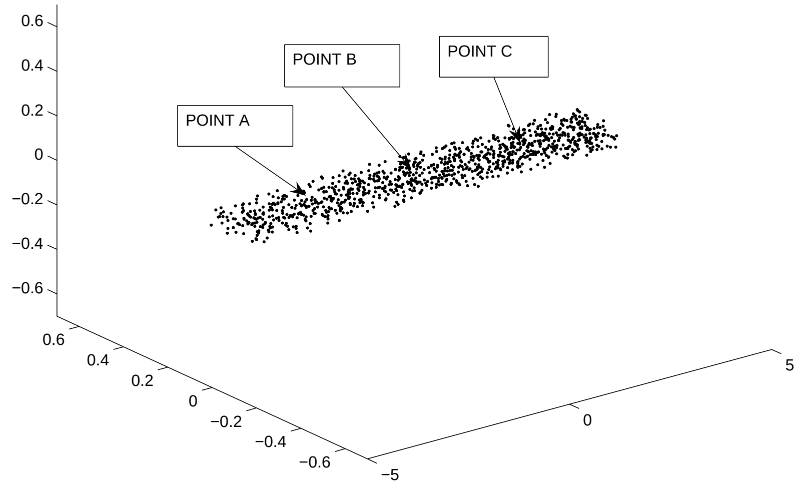
$$W = (V^T V)^{-1} V^T$$

  - If the encoder and decoder weights are tied $W = V^T$, the columns of the weight matrix V will become mutually orthogonal.
  - Easily shown by substituting $W = V^T$ above and postmultiplying with V to obtain $V^T V = I$.
  - This is exactly SVD!

- Tying encoder-decoder weights does not lead to orthogonality for other architectures, but is a common practice anyway.

Deep Autoencoders





- Better reductions are obtained by using increased depth and nonlinearity.

- Crucial to use nonlinear activations with deep autoencoders.

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Row-Index to Row-Value Autoencoders: Incomplete Matrix Factorization for Recommender Systems

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.6

Recommender Systems

- Recap of SVD: Factorizes $D \approx UV^T$ so that the sum-of-squares of residuals $||D - UV^T||^2$ is minimized.
  - Helpful to watch previous lecture on SVD
- In recommender systems (RS), we have an $n \times d$ ratings matrix D with n users and d items.
  - Most of the entries in the matrix are unobserved
  - Want to minimize $||D - UV^T||^2$ only over the observed entries
  - Can reconstruct the entire ratings matrix using $UV^T \Rightarrow$ Most popular method in traditional machine learning.

Difficulties with Autoencoder

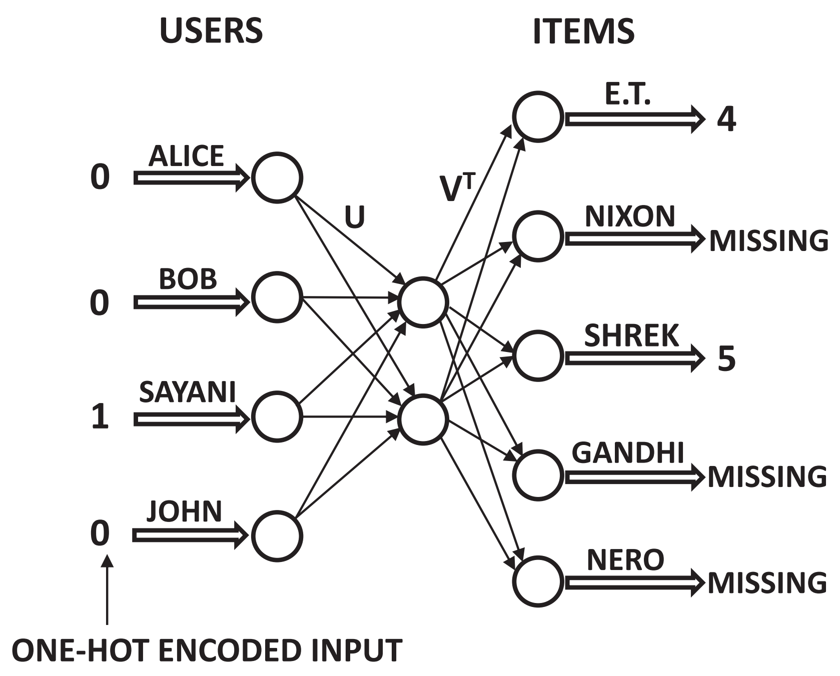
- If some of the inputs are missing, then using an autoencoder architecture will implicitly assume default values for some inputs (like zero).
  - This is a solution used in some recent methods like *AutoRec*.
  - Does not exactly simulate classical MF used in recommender systems because it implicitly makes assumptions about unobserved entries.

- None of the proposed architectures for recommender systems in the deep learning literature exactly map to the classical factorization method of recommender systems.

Row-Index-to-Row-Value Autoencoder

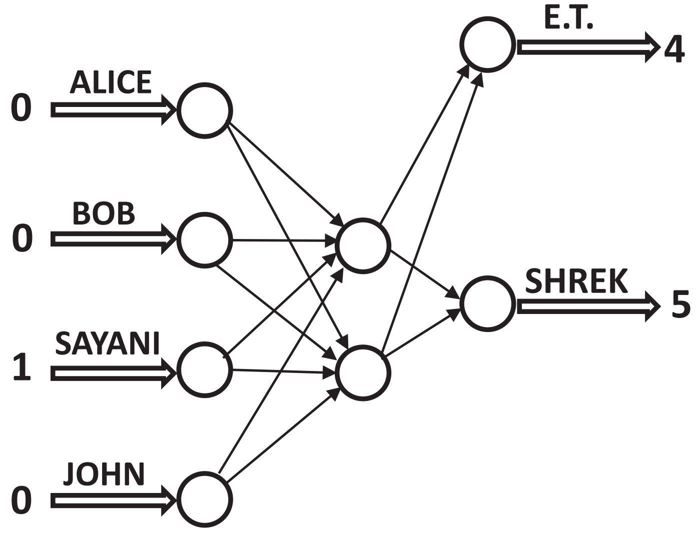
- Autoencoders map row values to row values.
  - Discuss an autoencoder architecture to map the one-hot encoded row *index* to the row values.
  - Not standard definition of autoencoder.
  - Can handle incomplete values but cannot handle out-of-sample data.
  - Also useful for representation learning (e.g., node representation of graph adjacency matrix).
- The row-index-to-row-value architecture is not recognized as a separate class of architectures for MF (but used often enough to deserve recognition as a class of MF methods).

Row-Index-to-Row-Value Autoencoder for RS

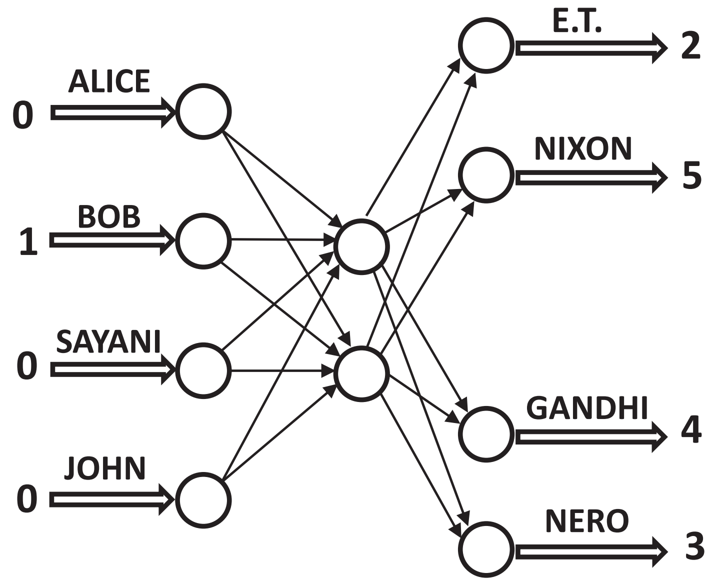


- Encoder and decoder weight matrices are U and V^T.
  - Input is one-hot encoded row index (only in-sample)
  - Number of nodes in hidden layer is factorization rank.
  - Outputs contain the ratings for that row index.

How to Handle Incompletely Specified Entries?



OBSERVED RATINGS (SAYANI): E.T., SHREK



OBSERVED RATINGS (BOB): E.T., NIXON, GANDHI, NERO

- Each user has his/her own neural architecture with missing outputs.

- Weights across different user architectures are shared.

Equivalence to Classical Matrix Factorization for RS

- Since the two weight matrices are U and V^T, the one-hot input encoding will pull out the relevant row from UV^T.

- Since the outputs only contain the observed values, we are optimizing the sum-of-square errors over observed values.

- Objective functions in the two cases are equivalent!

Training Equivalence

- For k hidden nodes, there are k paths between each user and each item identifier.

- Backpropagation updates weights along all k paths from each observed item rating to the user identifier.

  – Backpropagation in a later lecture.

- These k updates can be shown to be *identical* to classical matrix factorization updates with stochastic gradient descent.

- Backpropagation on neural architecture is identical to classical MF stochastic gradient descent.

Advantage of Neural View over Classical MF View

- The neural view provides natural ways to add power to the architecture with nonlinearity and depth.
  - Much like a child playing with a LEGO toy.
  - You are shielded from the ugly details of training by an inherent modularity in neural architectures.
  - The name of this magical modularity is backpropagation.
- If you have binary data, you can add logistic outputs for logistic matrix factorization.
- *Word2vec* belongs to this class of architectures (but *direct* relationship to nonlinear matrix factorization is not recognized).

Importance of Row-Index-to-Row-Value Autoencoders

- Several MF methods in machine learning can be expressed as row-index-to-row-value autoencoders (but not widely recognized–RS matrix factorization a notable example).

- Several row-index-to-row-value architectures in NN literature are also not fully recognized as matrix factorization methods.
  - The full relationship of *word2vec* to matrix factorization is often not recognized.
  - *Indirect* relationship to *linear* PPMI matrix factorization was shown by Levy and Goldberg.
  - In a later lecture, we show that *word2vec* is *directly* a form of *nonlinear* matrix factorization because of its row-index-to-row-value architecture and nonlinear activation.

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Word2vec: The Skipgram Model

Neural Networks and Deep Learning, Springer, 2018
Chapter 2, Section 2.7

Word2Vec: An Overview

- *Word2vec* computes embeddings of words using sequential proximity in sentences.
  - If *Paris* is closely related to *France*, then *Paris* and *France* must occur together in small windows of sentences.
    - Their embeddings should also be somewhat similar.
  - Continuous bag-of-words predicts central word from context window.
  - Skipgram model predicts context window from central word.

Words and Context

- A window of size t on either side is predicted using a word.

- This model tries to predict the context $w_{i-t}w_{i-t+1}\ldots w_{i-1}$ $w_{i+1}\ldots w_{i+t-1}w_{i+t}$ around word w_i, given the ith word in the sentence, denoted by w_i.

- The total number of words in the context window is $m = 2t$.

- One can also create a $d \times d$ word-context matrix C with frequencies c_{ij}.

- We want to find an embedding of each word.

Where have We Seen this Setup Before?

- Similar to recommender systems with *implicit feedback*.

- Instead of user-item matrices, we have square word-context matrices.

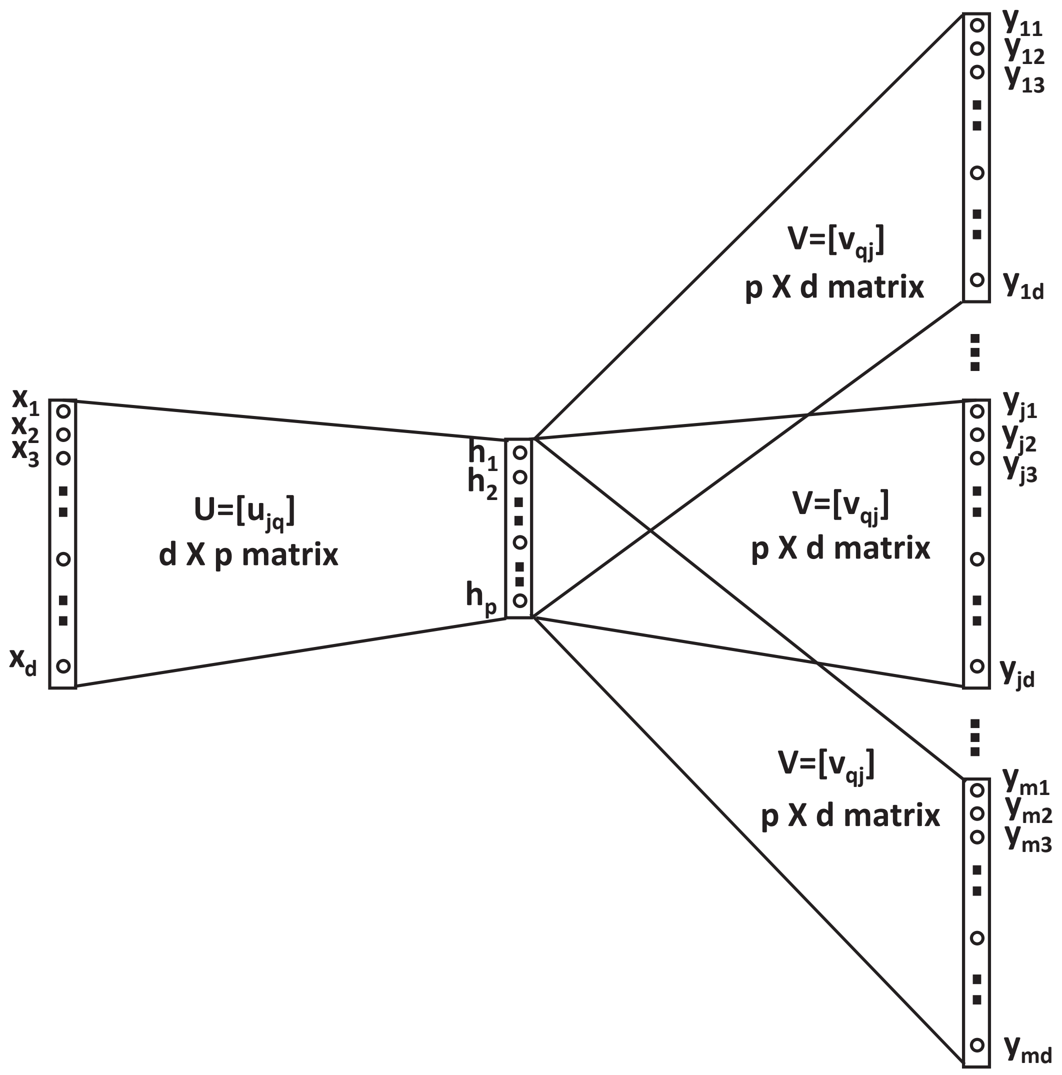
  - The frequencies correspond to the number of times a contextual word (column id) appears for a target word (row id).

  - Analogous to the number of units bought by a user (row id) of an item (column id).

  - An unrecognized fact is that skipgram *word2vec* uses an almost identical model to current recommender systems.

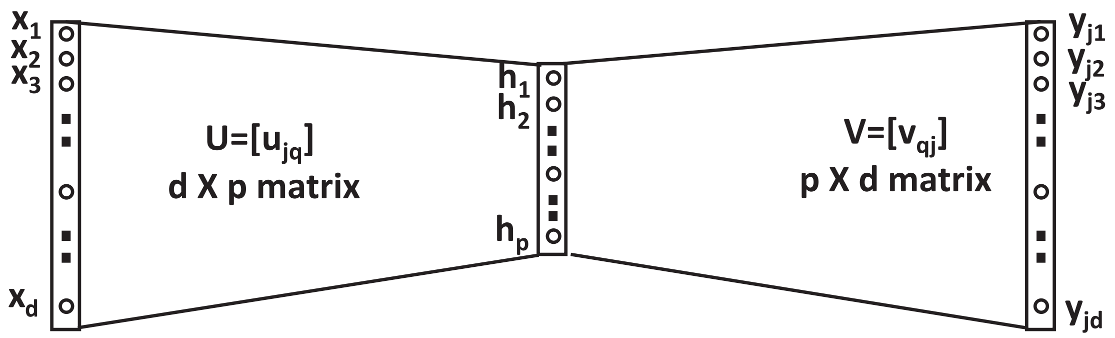
- Helpful to watch previous lecture on recommender systems with row-index-to-value autoencoders.

Word2Vec: Skipgram Model



- Input is the one-hot encoded word identifier and output contains m *identical* softmax probability sets.

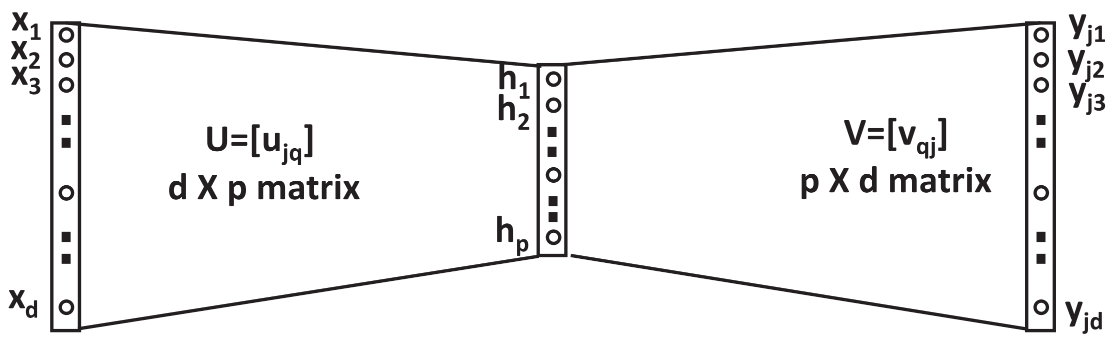
Word2Vec: Skipgram Model



MINIBATCH THE m d-DIMENSIONAL OUTPUT VECTORS IN EACH CONTEXT WINDOW DURING STOCHASTIC GRADIENT DESCENT. THE SHOWN OUTPUTS y_{jk} CORRESPOND TO THE jth OF m OUTPUTS.

- Since the m outputs are identical, we can collapse the m outputs into a single output.
- Mini-batch the words in a context window to achieve the same effect.
- Gradient descent steps for each instance are proportional to $d \Rightarrow$ Expensive.

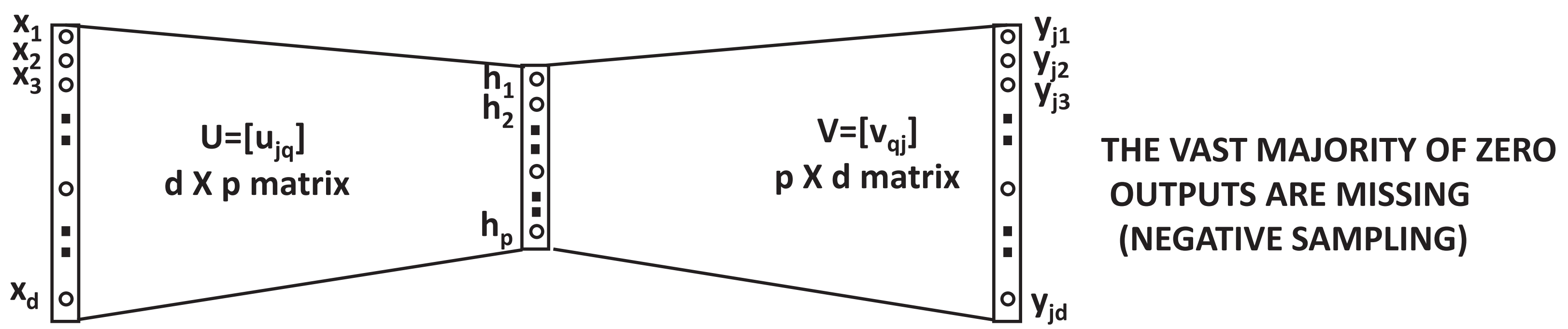
Word2Vec: Skipgram Model with Negative Sampling

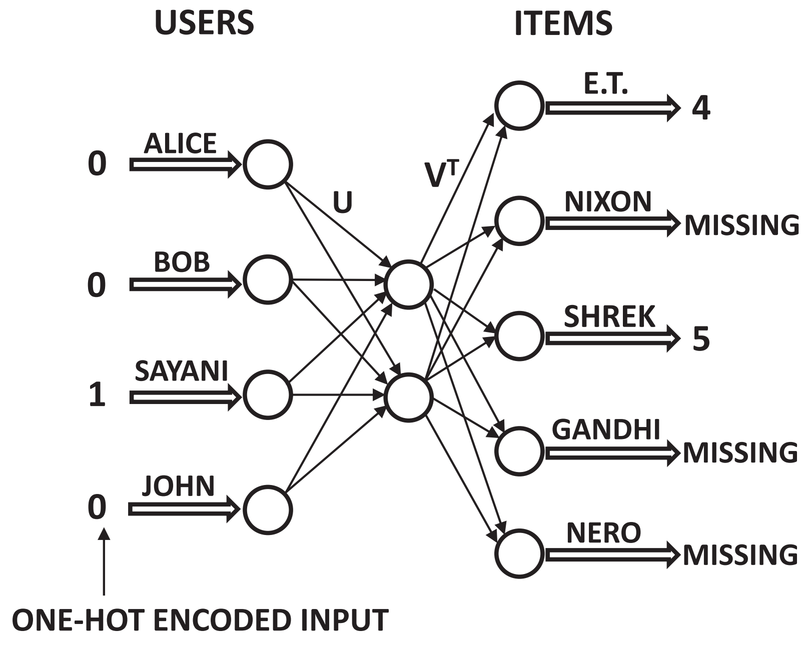


MINIBATCH THE m d-DIMENSIONAL OUTPUT VECTORS IN EACH CONTEXT WINDOW DURING STOCHASTIC GRADIENT DESCENT. THE SHOWN OUTPUTS y_{jk} CORRESPOND TO THE jth OF m OUTPUTS.

- Change the softmax layer into sigmoid layer.
- Of the d outputs, keep the positive output and sample k out of the remaining $d-1$ (with log loss).
- Where have we seen missing outputs before?

Can You See the Similarity?





- Main difference: Sigmoid output layer with log loss.

Word2Vec is Nonlinear Matrix Factorization

- Levy and Goldberg showed an *indirect* relationship between *word2vec* SGNS and PPMI matrix factorization.

- We provide a much more direct result in the book.
  - Word2vec is (weighted) logistic matrix factorization.
  - Not surprising because of the similarity with the recommender architecture.
  - Logistic matrix factorization is already used in recommender systems!
  - Neither the *word2vec* authors nor the community have pointed out this *direct* connection.

Other Extensions

- We can apply a row-index-to-value autoencoder to any type of matrix to learn embeddings of either rows or columns.

- Applying to graph adjacency matrix leads to node embeddings.

  - Idea has been used by *DeepWalk* and *node2vec* after (indirectly) enhancing the matrix entries with random-walk methods.

  - Details of graph embedding methods in book.