Module 4: Machine Learning

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Overview

Part I — Machine Learning

- Regression: Basics
- Kernel based regression: Radial Basis Function Networks and Gaussian Processes
- Single Hidden Layer (2-layer) Neural Networks

Part II - Deep Learning

- Classification, and the need to go beyond Gaussian kernel models
- Convolutional Neural Networks
- Implementation

Part III - Practical Deep Learning

- Keras/Pytorch Introduction
- Classification on a real dataset
- Unsupervised Learning
- RNNs and GANs

References

- Murphy Kevin, Machine Learning a Probabilistic Perspective [6]: A great primer on ML
- Goodfellow et al. Deep Learning [4]: Some details of state of the art
- The structure of this module: Lectures and slides in class by Girish; demos, experiments, and hacks by Karan

Notation

- y: Dependent variable, output variable, the variable to learn. $y \in \mathbb{R}$ for regression, or in $y \in \{-1,1\}$ for binary classification. y_i is the i^{th} training sample
- x: Independent variable, input variable. $x \in \mathbb{R}^n$ for regression, $x \in D$ for classification
- W, V: Weights
- \blacksquare θ : A generic container for weights, e.g. $\theta = [W, V]$
- **f** bases functions, not to be confused with f

Representing Knowledge

- Finding patterns in data
- \blacksquare Building models from data \rightarrow being able to predict patterns
- Deterministic vs Probabilistic models

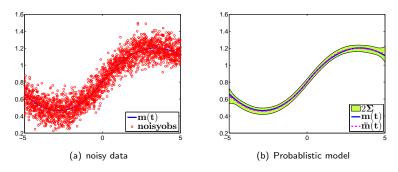


Figure:

Simple example: Curve fitting

- Consider that we are given a noisy data set $S = \{x_1, x_2, ..., x_N\}$
- Goal: Fit a curve for the given data: simple case: polynomial fit

$$y(x, w) = w_0 + w_1 x + w_2 x^2 + ... + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- acan write this in vector form: $y(x, w) = [1 \times x^2 \times x^3 \dots \times x^M]W$, where $W \in \Re^M$ is a column vector of weights
- Alternatively let $\phi(x) = [1 \times x^2 \times^3 \dots \times^M]^T$, then $y(x, W) = W^T \phi(x)$
- We can define a least squares error function:

$$E(W) = \frac{1}{2} \sum_{n=1}^{N} \{ (y(x_n, W) - W^{T} \phi(x_n))^{2} \}$$

 \blacksquare Agent can find weights W to minimize the cost function

Simple example

- Issues: what should be the dimension of W? \rightarrow the complexity of our model
- Will our approach handle noise?
- What other basis functions ϕ can I use?
- Heuristic: If the value of W is too high we will get overfitting
- solution: we can avoid overfitting through regularization: penalize high values in W:

$$\tilde{E}(w) = \frac{1}{2} \sum_{n=1}^{N} \{ (y(x_n, W) - W^T \phi(x_n))^2 \} + \frac{1}{2} \|W\|^2$$

- This still does not solve the problem of how to choose the number of parameters *M* in our model (too little, too much?)
- Bayesian (nonparametric) approach: adapt the number of parameters to the data
- Deep Neural Network approach: Use overparameterized models

Generalizing this idea

True function

Let $y \in \mathbb{R}$ be the dependent variable (scalar for now, but the idea generalizes immediately), and $x \in \mathbb{R}^n$ be the independent variable

$$y = f(x) \tag{1}$$

Is the true unknown function that satisfies some problem-specific guarantees

For $x \in \mathbb{R}^n$, let m be the number of "features", i.e. $\phi(x) \in \mathbb{R}^m$, and $W^* \in \mathbb{R}^m$ a vector of "ideal" weights

Universal Function approximation theorems NN [5], RBFN [8]

$$\|y(x) - W^{*T}\phi(x)\|_{\infty} < \epsilon(x)$$
 (2)

The Machine learning problem

Let $L(y(x), W^T \phi(x))$ be a loss function, let D be the set of N training inputs x_n then solve

$$W = \arg\min L(y(x_n), W^T \phi(x_n)) \forall x_n \in D$$
 (3)

Radial Basis function networks

Let $x \in \mathbb{R}^n$ be the independent variable, let $c_j \in \mathbb{R}^n$ be an "RBF center", then

Gaussian Radial Basis Functions

$$\phi(x,c_j) = e^{\frac{-\|x-c_j\|^2}{\sigma^2}} \tag{4}$$

Here σ is the bandwidth of the kernel (how fat the kernel is)

Let $\Phi(x) = [\phi(x, c_1), \phi(x, c_2), \cdots, \phi(x, c_m)]^T$ The Radial Basis Function Network (RBFN) is formulated as

RBFN

$$\hat{y}(x) = \sum_{j=1}^{m} w_i \phi(x, c_j) = W^T \Phi(x)$$
 (5)

Let $H = [y_1, y_2, \dots, y_N]^T$, $X = [\Phi(x_1), \Phi(x_2), \dots, \Phi(x_N)]^T$ and let $L(W, x) = ||y(x) - W^T \Phi(x)||_2^2$

Optimal (least-squares) solution for RBFN

$$W = \left[XX^{T} \right]^{-1} XH \tag{6}$$

Regularization

How do we prevent the Neural Network weights becoming "too big"?

Regularized Regression

$$L(W,x) = ||y(x) - W^T \Phi(x)||_2^2 + C||W||_2^2$$

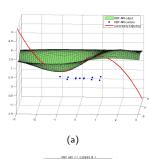
Solution

Optimal weights

$$W = \left[XX^T + CI \right]^{-1} XH$$

Gaussian Processes: "Broad" Bayesian RBFNs

- RBFs: linear-in-the-parameters, easier to analyze and easier to tune, more popular
- How many bases functions to use?
- How do I know my model is doing "good"?
- Gaussian Processes: Generalizing the idea of RBFN to accommodate potentially infinite number of bases functions





(b) A dimensional kernel one-

RBF

Reproducing Kernel Hilbert Spaces

- A Mercer Kernel $k(x_1, x_2) \in \mathbb{R}$ is a continuous, symmetric, positive definite function for $x_1, x_2 \in D \subset \mathbb{R}^n$
- Can think of kernels as a measure on similarity of any two points
- The Gaussian RBF is a Mercer kernel: $k(.,x_2)k(.,c_i) = \phi(.,c_i) = e^{\frac{-\|x-c_j\|^2}{\sigma^2}}$

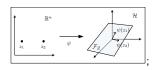


Figure: An example Hilbert space mapping.

(Mercer) RKHS

There exists a high (infinite) dimensional Hilbert space H and a mapping $\psi:D\to H$

■ Kernel trick: Although ψ may be unknown: $k(x_1, x_2) = \langle \psi(x_1), \psi(x_2) \rangle$

Gaussian Processes

- Idea: Starting from an infinite set of possible uncertainty representations, use data to narrow down the most applicable subset → Infer both the model structure and parameters from data
- Naive GP: add a kernel at every data point observed, i.e. add every x(t) to the set of centers $C = [c_1, c_2, \cdots, c_m]^T$
- Issue: Large computational burden (O(N³)) as data size increases, infeasible online
- Online sparsification: Only keep the most relevant kernels
 - Csato's online sparse GP [?]
 - Keep a buffer of most recent points

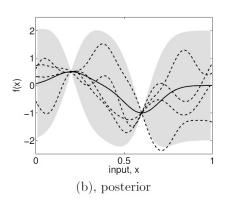


Figure: Posterior estimate given GP assumption

Gaussian Process Regression

- Let $X_t = \{x_1, \dots, x_t\}$ be a set of state measurements, with outputs $y_t(x_i) = f(x_i) + \epsilon_i$, where $\epsilon_i \sim \mathcal{N}(0, \omega^2)$ is Gaussian noise.
- Under GP model, data $\{f(x_1), \ldots, f(x_t)\}$ has prior distribution $\mathcal{N}(0, K(X_t, X_t))$, where $K(X_t, X_t)$ is Gram matrix of the elements in X_t .
- **C**an be shown that given a new input x_{t+1} , joint distribution of the data:

$$\begin{bmatrix} y_t \\ y_{t+1} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} K(X_t, X_t) + \omega^2 I & k_{x_{t+1}} \\ k_{x_{t+1}}^T & k_{t+1}^* \end{bmatrix} \right), \tag{7}$$

where $k_{x_{t+1}} = K(x_{t+1}, X_t)$ and $k_{t+1}^* = k(x_{t+1}, x_{t+1})$. Posterior:

$$p(y_{t+1}|X_t, y_t, x_{t+1}) \sim \mathcal{N}(\hat{m}_{t+1}, \bar{\Sigma}_{t+1}),$$
 (8)

where

$$\hat{m}_{t+1} = w_{t+1}^{\mathsf{T}} k_{\mathsf{x}_{t+1}} \tag{9}$$

$$\bar{\Sigma}_{t+1} = k_{t+1}^* - k_{x_{t+1}}^T C k_{x_{t+1}}$$
 (10)

are estimated mean and covariance respectively, and $C := (K(X_t, X_t) + \omega^2 I)^{-1}$ and $w_{t+1} := Cy_t$. Inversions can be computed recursively to improve computational efficiency

GPs as time-varying RBFNs

The key idea is that the set of centers can change with time

Naive: Add a center for every data point

Sparse: Use a fixed dictionary of centers and swap the centers out with the most

"useful" ones [3, 2]

Challenge

Well, we still haven't really solved the problem of how many kernels do we need, we just replaced it with creating a very large and flat model \rightarrow Broad networks

Stationary vs Non-stationary Kernel Functions

Maybe we can solve the problem by using more complicated kernels?

Stationary Squared Exponential (SE) Kernel: For $x_i, x_j \in \mathbb{R}^2$ $k(x_i, x_j) = \exp((x_i - x_j)^T \Sigma^{-1} (x_i - x_j))$

where $\Sigma = \sigma^2 \cdot \mathbf{I}_2$ is the covariance matrix,

■ Non-stationary SE Kernel [7]:

$$k(x_i, x_j) = |\Sigma_i|^{\frac{1}{4}} |\Sigma_j|^{\frac{1}{4}} |(\Sigma_i + \Sigma_j)/2|^{-\frac{1}{2}} \exp(-Q_{ij})$$
$$Q_{ij} = (x_i - x_j)^T ((\Sigma_i + \Sigma_j)/2)^{-1} (x_i - x_j),$$

 Σ_i is the covariance matrix at x_i , in isotropic case

$$\Sigma_i = \begin{bmatrix} \sigma_{(x_i)_1}^2 & 0\\ 0 & \sigma_{(x_i)_2}^2 \end{bmatrix}$$

- **Solving for** Σ_i : Computationally expensive MCMC sampling.
- Infeasible for massive scale data

Hierarchic Bayesian Models

- The general idea can be expanded to different distributions:
- Bayesian Nonparametrics: Model structure (number of parameters) and parameter values concurrently inferred from data [10, 9, 1]
- Attracting significant interest in the last 8-10 years

Model	Typical Application
GP	Learning continuous functions
DP	Mixture models
BP	Shared latent feature models
HDP-HMM	Hidden Markov models
HDP-SLDS-HMM	Hybrid system models
HDP-AR-HMM	
BP-AR-HMM	Hybrid system models with shared features
НВР	Mixtures of latent feature models

- Challenges: Computational scalability, on-line (sequential) implementation
- The Bayesian perspective is elegant, but practicality is limited due to MCMC (not the focus of this workshop)

Adaptive Basis Functions

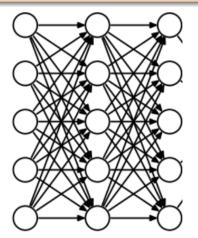
- Coming up with kernels is hard for general problems
- For regression, the Gaussian RBF does really well, in M3 we will show that it has some real power when dealing with smooth dynamical systems defined over continuous state-spaces
- But how do you build a kernel that compares two documents?
- Kernels that compare two images?
- There is another way: Adapt the features directly from the data
- That is learn filters that prioritize certain aspects of the data through some sort of a squashing function or gate

Remember me: Single Hidden Layer Neural Networks

There is another way of handling this problem

What if we went deep instead of broad?

$$y = W^T \sigma(V^T \bar{x})$$



A more detailed look

 W, V, \bar{x} are defined in the following:

- \blacksquare n_3 denote the number of output layer neurons ($n_3=1$ for scalar case)
- \blacksquare n_2 denote the number of hidden layer neurons
- \blacksquare n_1 denote the number of input layer neurons
- $W \in \Re^{(n_2+1) \times n_3}$ is the NN synaptic weight matrix connecting the hidden layer with the output layer
- $V \in \Re^{(n_1+1)\times n_2}$ is the NN synaptic weight matrix connecting the input layer with the hidden layer

Universal Approximation Theorem [5]

Given an $\bar{\epsilon} > 0$, for all $\bar{x} \in D$, where D is a compact set, there exists a number of hidden layer neurons n_2 , and an ideal set of weights (W^*, V^*) that brings the NN output to within an ϵ neighborhood of the function approximation error. The largest such ϵ is given by

$$\bar{\epsilon} = \sup_{\bar{x} \in D} \left\| W^{*^T} \sigma(V^{*^T} \bar{x}) - f(\bar{x}) \right\|. \tag{11}$$

More detailed look

The Output layer weight matrix W

$$W = \begin{pmatrix} \Theta_{w,1} & \cdots & \Theta_{w,n_3} \\ w_{1,1} & \cdots & w_{1,n_3} \\ \vdots & \ddots & \vdots \\ w_{n_2,1} & \cdots & w_{n_2,n_3} \end{pmatrix} \in \Re^{(n_2+1)\times n_3}, \tag{12}$$

The hidden layer weight matrix V

$$V = \begin{pmatrix} \Theta_{v,1} & \cdots & \Theta_{v,n_2} \\ v_{1,1} & \cdots & v_{1,n_2} \\ \vdots & \ddots & \vdots \\ v_{n_1,1} & \cdots & w_{n_1,n_2} \end{pmatrix} \in \Re^{(n_1+1)\times n_2}, \tag{13}$$

The input vector with a bias term \bar{x}

$$\bar{x} = \begin{pmatrix} b_{v} \\ x_{in} \end{pmatrix} = \begin{pmatrix} b_{v} \\ x_{in_{1}} \\ x_{in_{2}} \\ \vdots \\ x_{in_{n}} \end{pmatrix} \in \Re^{n_{1}+1}. \tag{14}$$

Continued detailed look

let $a=V^T\bar{x}\in\Re_2^n$, and b_w denote the constant bias term usually set to 1 for the hidden layer neuron. Then the vector function $\sigma(a)\in\Re^{n_2+1}$ is given by

$$\sigma(a) = \begin{pmatrix} b_w \\ \sigma_1(a_1) \\ \vdots \\ \sigma_{n_2}(a_{n_2}) \end{pmatrix} \in \Re^{n_2+1}. \tag{15}$$

The elements of σ consist of sigmoidal activation functions, in which c_j s are (different) constants

$$\sigma_j(\mathsf{a}_j) = \frac{1}{1 + \mathsf{e}^{-c_j \mathsf{a}_j}} \tag{16}$$

(17)

Alternative activation functions:

- \blacksquare tanh: $\sigma_i(a_i) = \tanh(a_i)$,
- RELU (Rectified Linear Activation Unit): $\sigma_i(a_i) = \max(0, a_i)$

Backpropagation

Genralize, let f denote σ (activation function)

Simplifying notation

$$\bar{x} \xrightarrow{V} a \xrightarrow{f} z \xrightarrow{W} b \xrightarrow{h} y$$

- $a = V^T \bar{x}$
- $z = f(a) = f(V^T \bar{x})$
- $b = W^T z = W^T \mathbf{f}(V^T \bar{x})$
- Assume h is identity
- Let $\theta = W, V$

Generic loss

Let $L(\theta)$ denote the generic loss, recall for regression Negative Log Likelihood:

$$L(\theta) = -\sum_{n} \sum_{k} (\hat{y}_{nk}(\theta) - y_{nk})^{2}$$

For (k-class) classification Negative Log Likelihood (more late):

$$L(\theta) = -\sum_{n} \sum_{k} y_{nk} \log \hat{y}_{nk}(\theta)$$

Backpropagation (Murphy pp 573[6])

■ We need $\nabla_{\theta} L$

Let's start at the output, noting $\frac{\partial b}{\partial W} = \frac{\partial W^T z}{\partial W} = z$

$$\nabla_W L = \frac{\partial L}{\partial b} \nabla_W b = \frac{\partial L}{\partial b} z \tag{18}$$

Now note that

$$\frac{\partial L}{\partial b} \triangleq \delta^{w} = (\hat{y} - y) \tag{19}$$

So the overall gradient is the input before applying **f** times the error:

$$\nabla_W L = \delta^W z \tag{20}$$

Now noting that $\nabla_V a = \frac{\partial a}{\partial V} = \frac{\partial V^T \bar{x}}{\partial V} = \bar{x}$:

$$\nabla_V L = \frac{\partial L}{\partial a} \nabla_V a \triangleq \delta^V \bar{x} \tag{21}$$

What we need now is δ^V , for this we "backpropagate" this error:

$$\delta^{v} = \frac{\partial L}{\partial a} = \frac{\partial L}{\partial b} \frac{\partial b}{\partial a} = \delta^{W} \frac{\partial b}{\partial a} \tag{22}$$

Backprop contd

Now
$$b = W^T z = W^T \mathbf{f}(a) = W^T \mathbf{f}(V^T \bar{x})$$
$$\frac{\partial b}{\partial a} = \frac{\partial W^T z}{\partial a} = \frac{\partial W^T \mathbf{f}(a)}{\partial a}$$

Which brings us to

$$\frac{\partial b}{\partial a} = \frac{\partial W' \mathbf{f}(a)}{\partial a} = W^{\mathsf{T}} \mathbf{f}'(a) \tag{23}$$

And now we can use the definitions: The elements of σ consist of sigmoidal activation functions, which are given by

$$\mathbf{f} = \sigma_j(\mathbf{a}_j) = \frac{1}{1 + e^{-c_j \mathbf{a}_j}} \tag{24}$$

$$\mathbf{f}' = \frac{\partial}{\partial \mathbf{a}_j} \sigma(\mathbf{a}_j) = \sigma_j(\mathbf{a}_j)(1 - \sigma_j(\mathbf{a}_j)) \tag{25}$$

Alternative activation functions:

- lacksquare tanh: $\mathbf{f}_j(a_j) = \tanh(a_j)$, $\frac{\partial}{\partial a_j} \mathbf{f}(a_j) = 1 \tanh^2(a_j)$
- RELU (Rectified Linear Activation Unit): $\mathbf{f}_j(a_j) = \max(0, a_j)$, its derivative is defined everywhere except at 0 as $\mathbf{f}_j'(a_j) = \begin{cases} 1, & \text{if } x > 0. \\ 0, & \text{otherwise.} \end{cases}$

Some NN activation functions

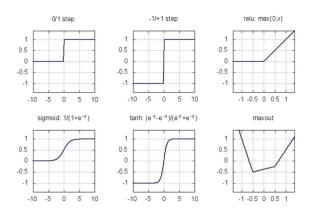


Figure: These ones are examples of squashers

(Figure: https://www.quora.com/Do-people-use-power-functions-like-x-3-or-x-5-as-activation-functions-in-artificial-neural-networks)

Logistic Regression

Question: How do we do classification ($y \in \{-1,1\}$) \Rightarrow Logistic Regression

Logistic Functions

Simple idea: Convert a linear function to a binary discriminator:

$$\mu(x) = \sigma(W^T x)$$

Where σ is a "squashing function". Examples:

- Sigmoidal
- tanh
- RELU

Probabilistic Intuition

$$p(y|x, W) = Ber(y|\mu(x))$$

where
$$\mu(x) = E[y|x] = p(y = 1|x)$$

Logistic Regression

Consider the binary classification problem $y=\{-1,1\}$ Then

$$p(y=1) = \frac{1}{1 + e^{-W^T \times}}$$

$$p(y=-1)=\frac{1}{1+e^{W^T \times}}$$

Hence

Negative Log Likelihood for Classification

$$L(W) = \sum_{i=1}^{N} \log(1 + e^{-y_i W^T x_i})$$

Cannot write down the Maximum Likelihood estimate in closed form \Rightarrow Stochastic gradient descent

$$W_{k+1} = W_k + \Gamma d_k$$

Where $d_k = -H_k^{-1}g_k$, and H_k is the Hessian, g_k is the gradient of L(w) (Murphy pp 249[6])

General Problem Formulation

Given a representer of the form $y = \mathbf{f}(\theta, x)$ and a generic loss function $L(\theta, x, y)$ solve

Generic ML problem

$$\min_{\theta} \sum_{x_i, y_i \in D} L(\mathbf{f}(\theta, x_i), y_i)$$

The generic loss function could also have robustifying terms, such as regularization: $\|\theta\|_2^2$

How should we choose **f**?

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- How should we choose f?
- We saw kernel models, they are great for regression, what about more general problems?
- We saw generic logistic regression problem, and its extension to the Single Hidden Layer network
- We noted we can "learn" θ using gradient descent, and backpropagate errors
- The idea we now explore is that of "adaptive data-driven bases", the essence of Deep Learning

PART II - Deep Learning

What function f(w, x, y) to choose?

What function f(w, x, y) to choose?

■ Choose any differentiable composite function

$$\mathbf{f}(w, x, y) = f_1(w_1, y, f_2(w_2, f_3(\dots f_n(w_n, x) \dots)))$$

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- Soft-max layer

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- Convolutions
- Rectified linear units max{0, x}
- Maximum-/Average pooling
- Fully connected layers
- Soft-max layer
- Dropout

Why go deep?

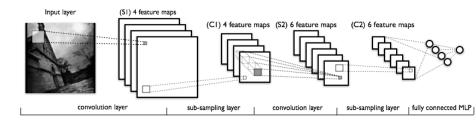
- Formal explanation: Our invited speaker R. Srikant will elaborate some results
- Somewhat formal: Point to Hornik's result and wave hands
- Informal: Adaptive features are extracted from data
- Essentially from a perspective of build gates, e.g. $\sigma(a)$ for the sigmoidal squasher, or $\mathbf{f} = \max(0, x)$ for the RELU

Example function architecture:

LeNet (LeCun 98)

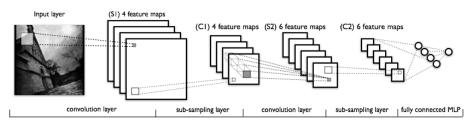
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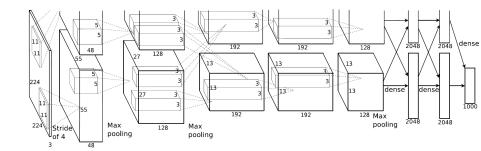
LeNet (LeCun 98)



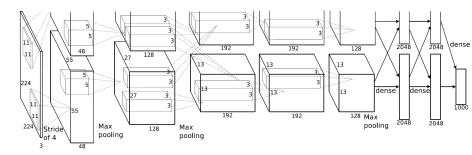
Decreasing spatial resolution and the increasing number of channels

Example function architecture: AlexNet

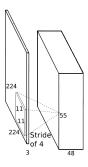
Example function architecture: AlexNet



Example function architecture: AlexNet



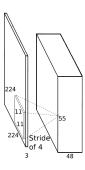
Decreasing spatial resolution and the increasing number of channels



120	190	140	150	200
17	21	30	8	27
89	123	150	73	56
10	178	140	150	18
190	14	76	69	87



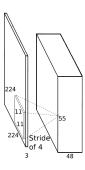
	98	98	



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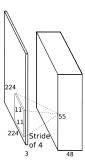




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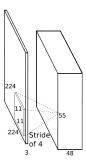




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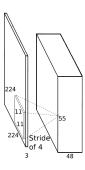




120	190	140	150	200	
17	21	30	8	27	
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190	14	76	69	87	

	1/9	1/9	1/9	
×	1/9	1/9	1/9	
	1/9	1/9	1/9	

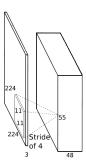




120	190	140	150	200
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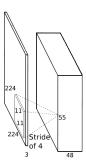
	98	98	93	
	84	97	72	
	108			



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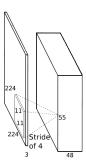
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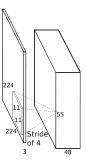
	1/9	1/9	1/9	
×	1/9	1/9	1/9	
	1/9	1/9	1/9	

98	98	93	
84	97	72	
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120	190	140	150	200										
17	21	30	8	27		1/9	1/9	1/9			98	98	93	
89	123	150	73	56	×	1/9	1/9	1/9	-		84	97	72	
10	178	140	150	18		1/9	1/9	1/9			108	108	91	
190	14	76	69	87										Γ
	17 89 10	17 21 89 123 10 178	17 21 30 89 123 150 10 178 140	17 21 30 8 89 123 150 73 10 178 140 150	17 21 30 8 27 89 123 150 73 56 10 178 140 150 18	17 21 30 8 27 89 123 150 73 56 x 10 178 140 150 18	17 21 30 8 27 1/9 89 123 150 73 56 x 1/9 10 178 140 150 18	17 21 30 8 27 1/9 1/9 89 123 150 73 56 x 1/9 1/9 10 178 140 150 18 1/9 1/9	17 21 30 8 27 1/9 1/9 1/9 89 123 150 73 56 x 1/9 1/9 1/9 10 178 140 150 18 1/9 1/9 1/9	17 21 30 8 27 1/9 1/9 1/9 89 123 150 73 56 x 1/9 1/9 1/9 = 10 178 140 150 18	17 21 30 8 27 1/9 1/9 1/9 89 123 150 73 56 x 1/9 1/9 1/9 = 10 178 140 150 18	17 21 30 8 27 1/9 1/9 1/9 98 98 123 150 73 56 X 1/9 1/9 1/9 1/9 = 84 10 178 140 150 18 1/9 1/9 1/9 1/9 1/9 108	17 21 30 8 27 1/9 1/9 1/9 1/9 98 98 98 99 123 150 73 56 X 1/9 1/9 1/9 1/9 1/9 1/9 1/9 1/9 1/9 1/9	17 21 30 8 27 1/9 1/9 1/9 98 98 93 93 123 150 73 56 x 1/9 1/9 1/9 1/9 84 97 72 10 178 140 150 18

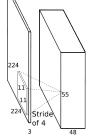
Trainable parameters w:



120	190	140	150	200	
17	21	30	8	27	
89	123	150	73	56	
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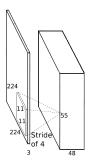
Trainable parameters w:

Filters (width, height, depth, number)

120	190	140	150	200	
17	21	30	8	27	
89	123	150	73	56	
10	178	140	150	18	
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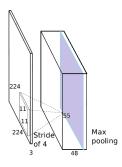
	1/9	1/9	1/9	
x	1/9	1/9	1/9	
	1/9	1/9	1/9	

98	98	93	
84	97	72	
108	108	91	

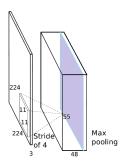


Trainable parameters w:

- Filters (width, height, depth, number)
- Bias

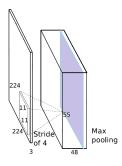


Maximum or average over a spatial region



Maximum or average over a spatial region

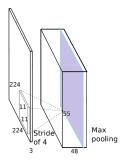
Trainable parameters w:

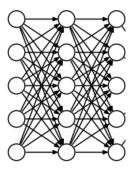


Maximum or average over a spatial region

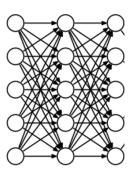
Trainable parameters w:

None



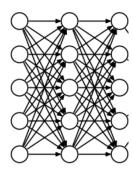






$$Wx + b$$

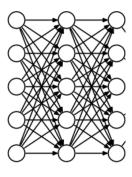
Trainable parameters w:



$$Wx + b$$

Trainable parameters w:

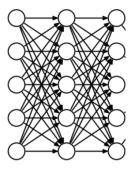
■ Matrix



$$Wx + b$$

Trainable parameters w:

- Matrix
- Bias



Soft-max layer:

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$$x \longrightarrow \frac{\exp x_i}{\sum_j \exp x_j}$$

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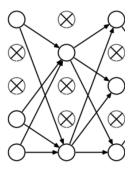
Trainable parameters w:

Soft-max layer:

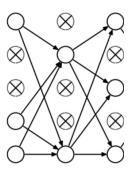
$$x \longrightarrow \frac{\exp x_i}{\sum_j \exp x_j}$$

Trainable parameters w:

None

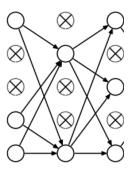


Randomly drop some activations



Randomly drop some activations

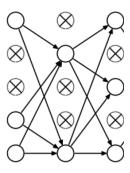
Trainable parameters w:



Randomly drop some activations

Trainable parameters w:

None



$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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Often also referred to as maximizing the regularized cross entropy:

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Often also referred to as maximizing the regularized cross entropy:

$$\max_{w} -\frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \sum_{\hat{y}} p_{\mathsf{GT}}^{(i)}(\hat{y}) \ln p(\hat{y}|x)$$
 with

$$\min_{w} \frac{C}{2} ||w||_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{v}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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What is C?

$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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What is C? Weight decay (aka regularization constant)

$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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What is C? Weight decay (aka regularization constant)

How to optimize this?

$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

Often also referred to as maximizing the regularized cross entropy:

$$\max_{\mathbf{w}} - \frac{C}{2} \|\mathbf{w}\|_{2}^{2} + \sum_{i \in \mathcal{D}} \sum_{\hat{\mathbf{y}}} p_{\mathsf{GT}}^{(i)}(\hat{\mathbf{y}}) \ln p(\hat{\mathbf{y}}|\mathbf{x}) \quad \text{with} \quad \left\{ \begin{array}{lcl} p_{\mathsf{GT}}^{(i)}(\hat{\mathbf{y}}) & = & \delta(\hat{\mathbf{y}} = \mathbf{y}^{(i)}) \\ p(\hat{\mathbf{y}}|\mathbf{x}) & \propto & \exp F(\mathbf{w}, \mathbf{x}, \hat{\mathbf{y}}) \end{array} \right.$$

What is C? Weight decay (aka regularization constant)

How to optimize this?

Stochastic gradient descent with momentum: What was this again?

Since F(w, x, y) is no longer constrained in any form, the loss function is generally no longer convex.

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Implications:

Since F(w, x, y) is no longer constrained in any form, the loss function is generally no longer convex.

Implications:

■ We are no longer guaranteed to find the global optimum

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Implications:

- We are no longer guaranteed to find the global optimum
- Initialization of w matters

$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

is?

$$\min_{w} \frac{C}{2} \|w\|_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{v}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

is?

$$Cw + \sum_{i \in \mathcal{D}} \sum_{\hat{y}} \left(p(\hat{y}|x) - \delta(\hat{y} = y^{(i)}) \right) \frac{\partial F(w, x, \hat{y})}{\partial w}$$

$$\min_{w} \frac{C}{2} ||w||_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

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$$p(\hat{y}|x) = \frac{\exp F(w,x,\hat{y})}{\sum_{\vec{y}} \exp F(w,x,\tilde{y})}$$
 via soft-max which takes F as input

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- $p(\hat{y}|x) = \frac{\exp F(w,x,\hat{y})}{\sum_{\vec{y}} \exp F(w,x,\tilde{y})}$ via soft-max which takes F as input
 - A dedicated cross-entropy layer exists (numerically more stable)

$$\min_{w} \frac{C}{2} ||w||_{2}^{2} + \sum_{i \in \mathcal{D}} \ln \sum_{\hat{y}} \exp F(w, x, \hat{y}) - F(w, x, y^{(i)})$$

is?

$$Cw + \sum_{i \in \mathcal{D}} \sum_{\hat{y}} \left(p(\hat{y}|x) - \delta(\hat{y} = y^{(i)}) \right) \frac{\partial F(w, x, \hat{y})}{\partial w}$$

- $p(\hat{y}|x) = \frac{\exp F(w,x,\hat{y})}{\sum_{\vec{y}} \exp F(w,x,\tilde{y})}$ via soft-max which takes F as input
 - A dedicated cross-entropy layer exists (numerically more stable)
- $\frac{\partial F(w,x,\hat{y})}{\partial w}$ via backpropagation

$$F(w,x,y) = f_1(w_1, f_2(w_2, f_3(w_3, x)))$$
 with activations
$$\begin{cases} x_2 = f_3(w_3, x) \\ x_1 = f_2(w_2, x_2) \end{cases}$$

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What is
$$\frac{\partial F(w,x,y)}{\partial w_3}$$
?

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$$\frac{\partial F(w,x,y)}{\partial w_3}$$
?
$$\frac{\partial f_1}{\partial x_1} \cdot \frac{\partial x_1}{\partial x_2} \cdot \frac{\partial x_2}{\partial w_3} =$$

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$$F(w,x,y) = f_1(w_1, f_2(w_2, f_3(w_3, x)))$$
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$$\frac{\partial f_1}{\partial x_1} \cdot \frac{\partial x_1}{\partial w_2} =$$

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$$\frac{\partial f_1}{\partial x_1} \cdot \frac{\partial x_1}{\partial w_2} = \frac{\partial f_1}{\partial f_2} \cdot \frac{\partial f_2}{\partial w_2}$$

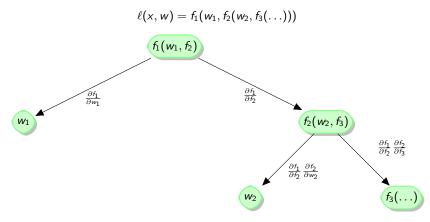
$$F(w,x,y) = f_1(w_1, f_2(w_2, f_3(w_3, x))) \text{ with activations } \begin{cases} x_2 = f_3(w_3, x) \\ x_1 = f_2(w_2, x_2) \end{cases}$$

What is
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$$\frac{\partial f_1}{\partial x_1} \cdot \frac{\partial x_1}{\partial x_2} \cdot \frac{\partial x_2}{\partial w_3} = \frac{\partial f_1}{\partial f_2} \cdot \frac{\partial f_2}{\partial f_3} \cdot \frac{\partial f_3}{\partial w_3}$$

What is
$$\frac{\partial F(w,x,y)}{\partial w_2}$$
?
$$\frac{\partial f_1}{\partial x_1} \cdot \frac{\partial x_1}{\partial w_2} = \frac{\partial f_1}{\partial f_2} \cdot \frac{\partial f_2}{\partial w_2}$$

Generally: To avoid repeated computation, backpropagation on a directed acyclic graph.

Composite function represented as a directed a-cyclic graph



Repeated application of chain rule for efficient computation of all gradients

A deep net with a single fully connected layer is equivalent to logistic regression

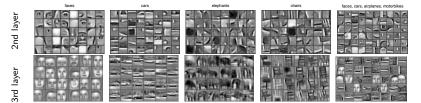
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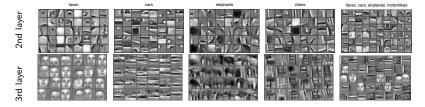
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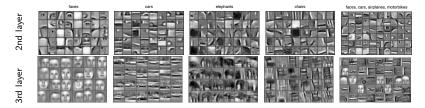
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Disadvantage of deep nets compared to usage of features:

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Disadvantage of deep nets compared to usage of features:

Deep nets are computationally demanding (GPUs) and require significant amounts of training data

■ Sufficient computational resources

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- Sufficient data

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- Sufficient algorithmic advances

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This combination lead to significant performance improvements on many datasets

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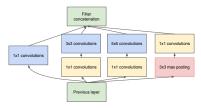
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 - Normalize by subtracting mean and dividing by standard deviation

LeNet

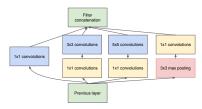
- LeNet
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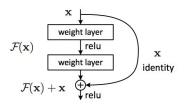
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- GoogLeNet (inception module)



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■ ResNet (residual connections)



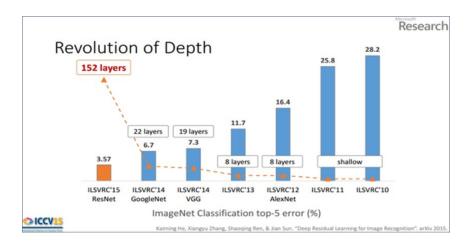
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Results:

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