Lecture 13

Neural Networks

ESL 11.3 – 11.7

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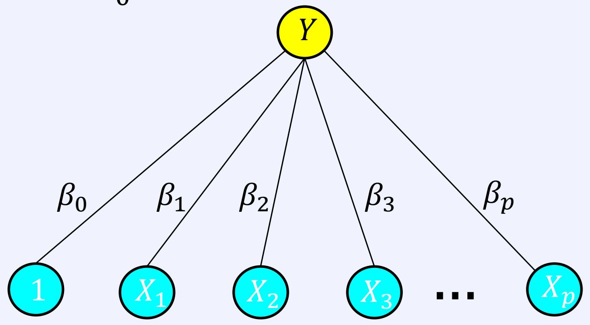
Another look at (Logistic) Regression

The model is $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$

- equivalently $Y = \beta_0 + \beta^T X$ where β and X are now vectors
- equivalently $Y = \beta^T X$ for an X where we added a constant feature $X_0 = 1$



For binary classification we apply the sigmoid function σ

- $Y = \sigma(\beta_0 + \beta^T X)$
- σ squishes the output between 0 and 1
- Y can be interpreted as the probability of class 1

We can only model linear functions!

Introducing Non-linearity

General recipe: transform $\boldsymbol{X}$ into some other space $\boldsymbol{Z}$ and fit a linear model on $\boldsymbol{Z}$

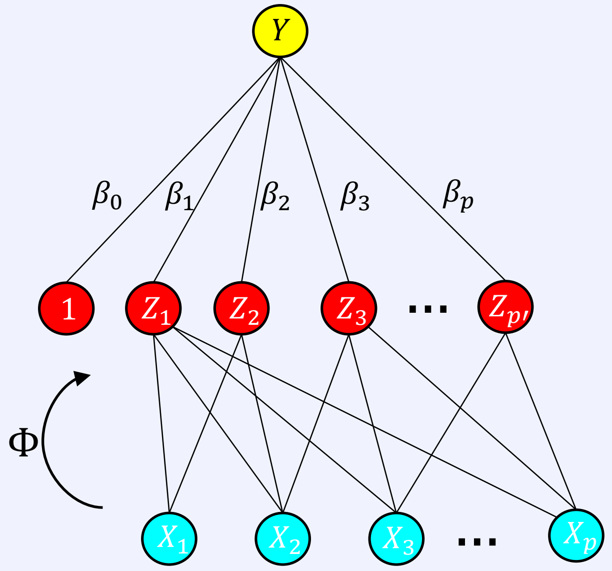
Polynomial regression: add higher-order terms

- $X_1, \mathrm{X}_1^2, X_2, \mathrm{X}_2^2, \dots, X_p, \mathrm{X}_p^2$
- rename $Z_1 = X_1,\ Z_2 = \mathrm{X}_1^2,\ Z_3 = X_2, \dots, Z_{p'} = X_p^2$
- we can have interaction terms, e.g. $Z_i = X_2 \cdot X_5$

SVM: apply a kernel $K(\cdot,\cdot)$ equivalent to a transformation $\boldsymbol{\Phi}$

- $Z = \Phi(X)$ is now the RKHS (that we called $\boldsymbol{\Psi}$ in previous lecture)

These transformations are fixed. Why don't we learn them?



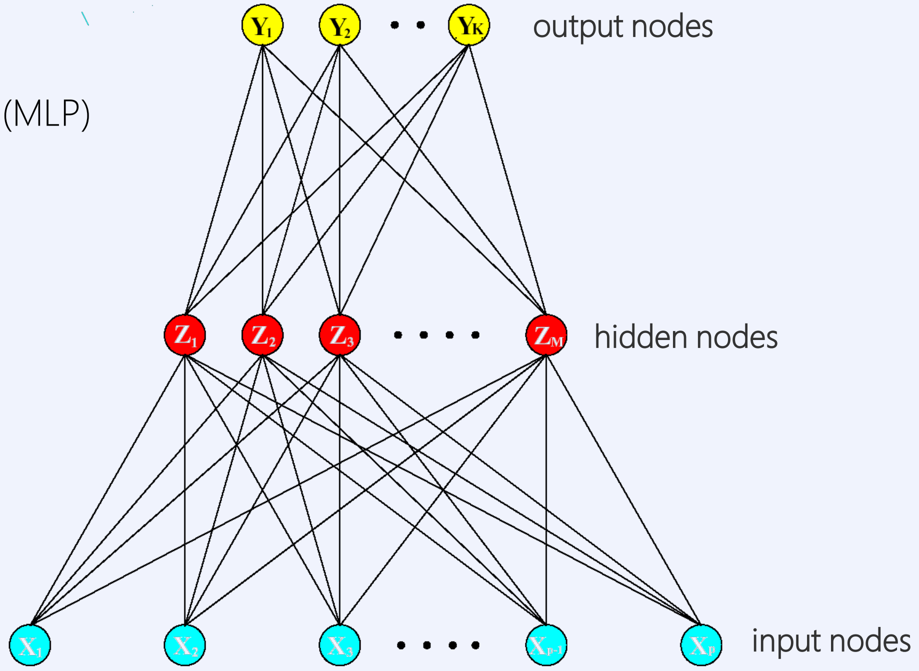
Neural Networks

Single hidden layer neural network

- aka feed-forward NN, aka multilayer perceptron (MLP)
- represented by a network diagram

Works for regression and classification

- regression: typically $K = 1$ but we can handle multiple quantitative responses
- K-class classification: K output units, where Y_k models the probability of class k



Neural Networks

The **derived (hidden) features** are defined as

$Z_m = \sigma(\alpha_{0m} + \alpha_m^T X), \quad m = 1, \dots, M$

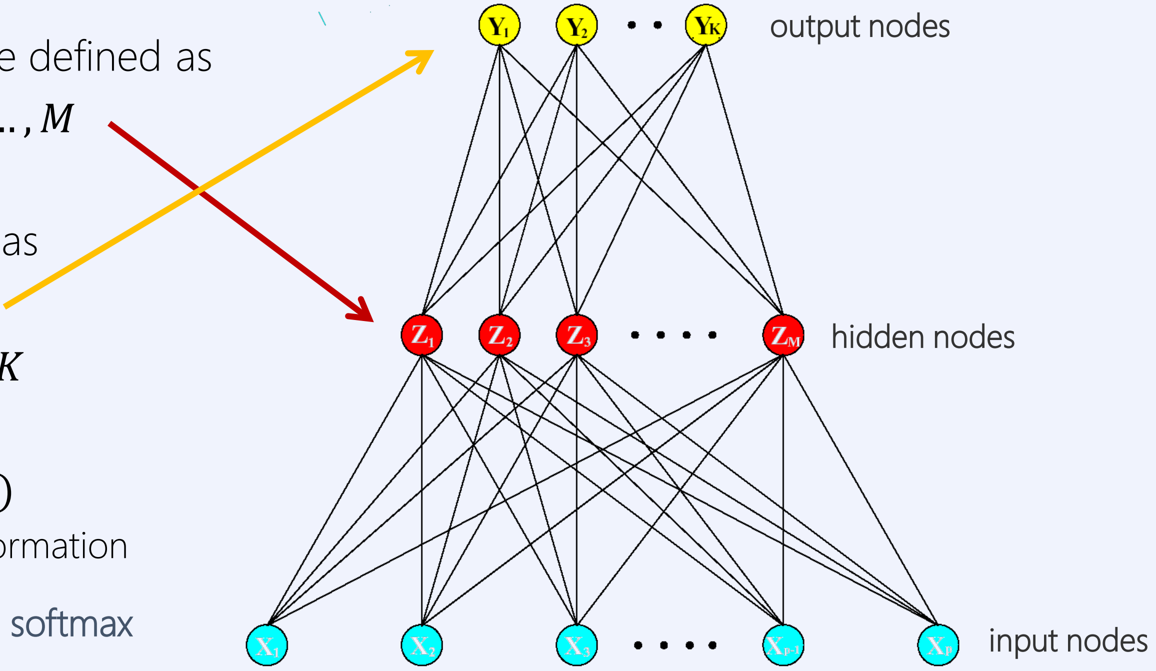
The **output features** are defined as

$T_k = \beta_{0k} + \beta_k^T Z, k = 1, \dots, K$

$Y_k = f_k(X) = g_k(T), \; k = 1, \dots, K$

The output transformation $g_k(T)$

- regression $g_k(T) = T_k$, no transformation
- classification $g_k(T) = \frac{e^{T_k}}{\sum_{l=1}^{K} e^{T_l}}$, the softmax ensures Y_k are positive and sum to 1



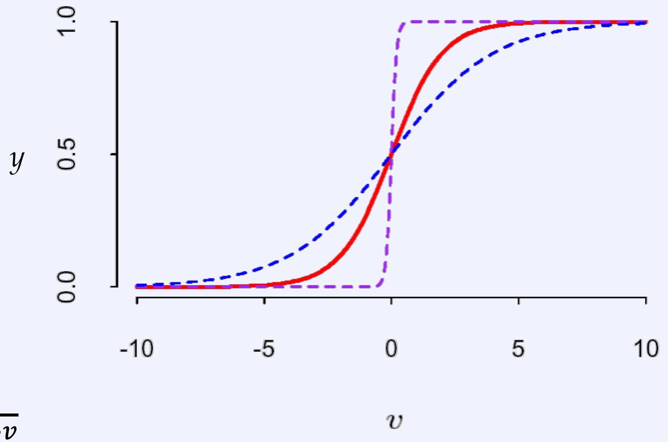
The activation function σ

Why do we need an activation function?

- ignoring the bias we have $Z_m = \sigma(\alpha_m^T X)$ and $T_k = \beta_k^T Z$

If σ is the identity function then

- $T_k = \beta_k^T Z = \beta_k^T(\alpha_m^T X)$
- equivalent to $T_k = \tilde{\beta} Z$ for some $\tilde{\beta}$
- the final model is still linear



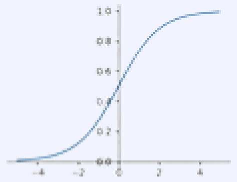
A useful activation function is the sigmoid $\sigma(v) = \frac{1}{1+e^{-v}}$

- each hidden node projects the data along a specific direction α_m and applies a sigmoid along this direction
- $\sigma(s(v - v_0))$ shifts the inflection point from 0 to v_0 and scales the function by a factor s

Activation functions

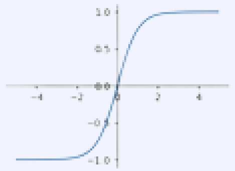
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



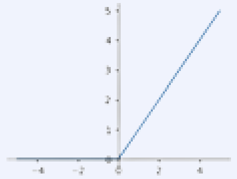
tanh

$$\tanh(x)$$



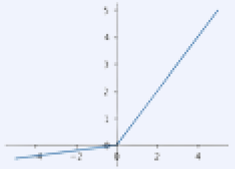
ReLU

$$\max(0, x)$$



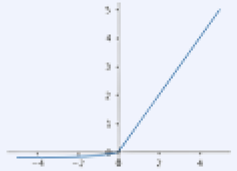
Leaky ReLU

$$\max(0.1x, x)$$



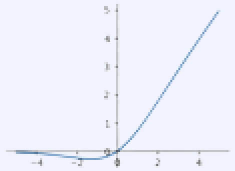
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Swish

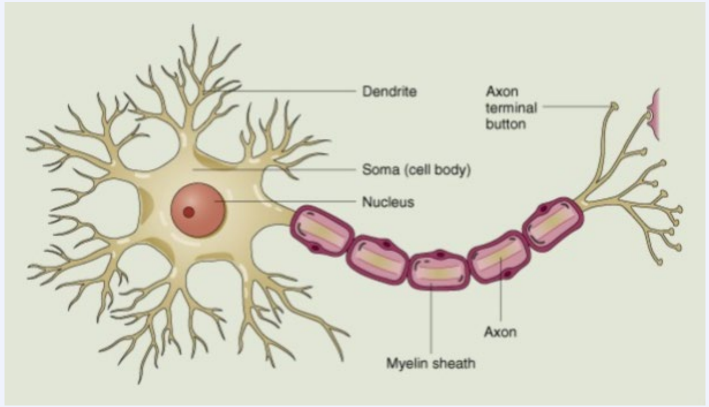
$$x \cdot \sigma(x)$$



Naming of Neural Networks

Naming from (loose) analogy to neurons in the brain

- **dendrites** receive analog input (post-synaptic potentials)
- the **soma** integrates these potentials
- if result exceeds a threshold it fires a sequence of spikes (action potentials) down the **axon**
- firing frequency rises with the total potential
- arrival of a spike at the **axon terminal** causes **neurotransmitter** to be released into the **synaptic cleft**.
- higher frequency of spikes = more transmitter released



Originally the activation function σ was a step function realizing a firing threshold

- was not appropriate for optimization

Fitting a Neural Network

The unknown parameters of a neural net (NN) are the sets of weights θ

- $\{\alpha_{0m}, \alpha_m; m = 1,2,\ldots,M\}$ $\quad M(p+1)$
- $\{\beta_{0k}, \beta_k; k = 1,2,\ldots,K\}$ $\quad K(M+1)$

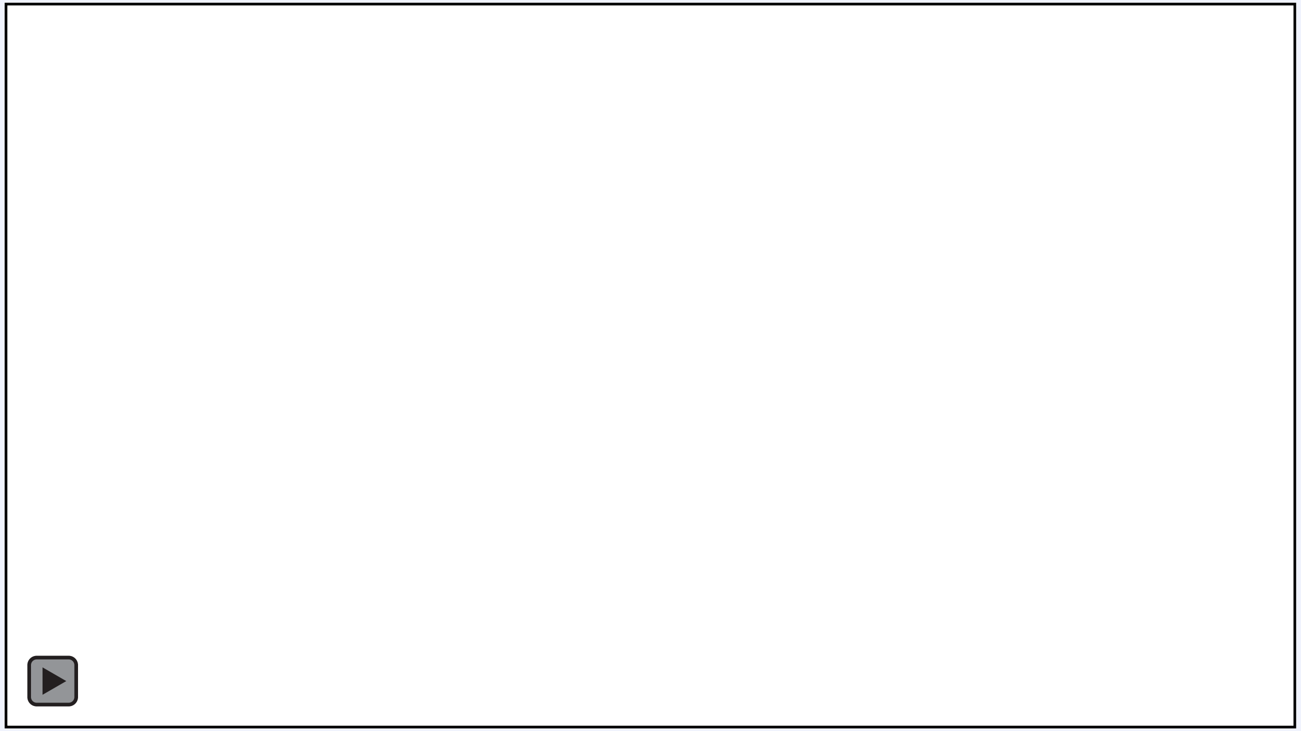
Regression: typically use sum of squares as error measure $R(\theta) = \sum_{i=1}^{N} \sum_{k=1}^{K} \left(y_{ik} - f_k(x_i)\right)^2$

Classification: typically use cross entropy $R(\theta) = -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{ik} \log f_k(x_i)$

- with the final classifier as $\arg\max_k f_k(x)$

With softmax and cross entropy a NN equals a linear logistic regression model in its hidden units, but the overall model is non-linear since Z is a non-linear transformations of X

The Sound of Machine Learning that is just



logistic regression...

(credits @MaartenvSmeden)

Fitting a Neural Network

All parameters are estimated by maximum likelihood

The global minimizer is likely to overfit the data, thus we need regularization

- through a penalty term or
- by early stopping

Training by gradient descent is now called back propagation

- detailed for square-error loss in the next slide

Recall the chain rule: for $f(x) = d(c(b(a(x))))$ we have:

$$\frac{\partial f}{\partial x} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial x}$$

Fitting a Neural Network

The model definition:

- $Z_m = \sigma(\alpha_{0m} + \alpha_m^T X),\ m = 1, .., M$
- $T_k = \beta_{0k} + \beta_k^T Z,$ and $Y_k = f_k(X) = g_k(T), k = 1, \dots, K$

So we have $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i),\ z_i = (z_{1i}, z_{2i}, \dots, z_{Mi}),\ i = 1, \dots, N$

The error is $R(\theta) = \sum_{i=1}^N R_i = \sum_{i=1}^N \sum_{k=1}^K \big(y_i - f_k(x_i)\big)^2$ with the derivative as

$$\frac{\partial R_i}{\partial \beta_{km}} = -2\big(y_{ik} - f_k(x_i)\big) g_k'\big(\beta_k^T z_i\big) z_{mi}$$

$$\frac{\partial R_i}{\partial \alpha_{ml}} = -\sum_{k=1}^{K} 2\big(y_{ik} - f_k(x_i)\big) g_k'\big(\beta_k^T z_i\big) \beta_{km} \sigma'(\alpha_m^T x_i) x_{il}$$

(Rumelhart et al, 1986) 12

Fitting a Neural Network

- $\frac{\partial R_i}{\partial \beta_{km}} = \underbrace{-2\big(y_{ik} - f_k(x_i)\big)g_k'\big(\beta_k^T z_i\big)}_{\delta_{ki}} z_{mi}$ $\qquad (*)$
- $\frac{\partial R_i}{\partial \alpha_{ml}} = \underbrace{-\sum_{k=1}^{K} 2\big(y_{ik} - f_k(x_i)\big)g_k'\big(\beta_k^T z_i\big)\beta_{km}\sigma'(\alpha_m^T x_i)}_{s_{mi}} x_{il}$

We use the gradients in the following gradient descent formula where γ_r is the learning rate

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \partial R_i / \partial \beta_{km}^{(r)}$$

$$\alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \partial R_i / \partial \alpha_{ml}^{(r)}$$

back propagation equations

By $(*)$ the derivatives have the simplified form $\frac{\partial R_i}{\partial \beta_{km}} = \delta_{ki} z_{mi}$ and $\frac{\partial R_i}{\partial \alpha_{ml}} = s_{mi} x_{il}$

where δ_{ki} and s_{mi} are the current error terms and satisfy $s_{mi} = \sigma'(\alpha_m^T x_i) \sum_{k=1}^{K} \beta_{km} \delta_{ki}$

(Rumelhart et al, 1986)

Fitting a Neural Network

The gradient descent updates are

- $\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \partial R_i / \partial \beta_{km}^{(r)}$ and $\alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \partial R_i / \partial \alpha_{ml}^{(r)}$ $(**)$
- with derivatives $\frac{\partial R_i}{\partial \beta_{km}} = \delta_{ki} z_{mi}$ and $\frac{\partial R_i}{\partial \alpha_{ml}} = s_{mi} x_{il}$

The updates in $(**)$ can be done by a two-pass algorithm

1. Forward pass
   - fix current weights and compute the predicted output values Y_k
2. Backward pass
   - compute the errors δ_{ki}
   - "back propagate" the errors to obtain the values s_{mi}
   - use these values to compute the gradients and do the update $(**)$

Training with the cross entropy error is analogous

(Rumelhart et al, 1986)

Remarks on Backpropagation

Backpropagation is local in nature

- every weight depends only on the weights of neurons connected to the respective neuron
- the algorithm hence allows for trivial parallelization

We discussed (full) batch learning, where all training data is processed simultaneously

- there is also an online version where training data is fed continually in a repeating cycle
- great for very large training sets
- stochastic gradient descent on mini-batches of data

- larger batch $\Rightarrow$ less noise in the gradient estimate
- but some noise can be good, e.g. act as a regularizer and help us escape bad local minima

(Robbins & Munro, 1951) (ESL 11.4)

Remarks on Backpropagation

Learning rate γ_r usually a constant

- can be optimized by a line search along the direction of the gradient
- should decrease to 0 in online setting
- variant of stochastic approximation, ensures convergence if $\gamma_r \to 0,\ \sum_r \gamma_r = \infty,\ \sum_r \gamma_r^2 < \infty$
- first-order methods can be very slow, sadly, Newton's method is not appropriate since the second derivative of R can be very large

Backpropagation is not just the chain rule, with automatic differentiation (Pytorch, Tensorflow)

- it is a particularly efficient strategy for computing the chain rule
- evaluating $\nabla f(x)$ provably as fast as evaluating $f(x)$
- code for $\nabla f(x)$ can be automatically derived even if we have control flow structures like loops
- it operates on a more general family of functions: programs which have intermediate variables

Issues with Training

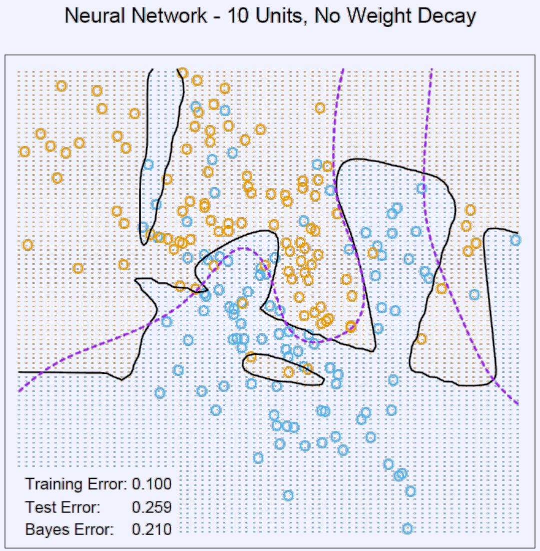
Starting values – initialization of the parameters

- large initial weights usually lead to poor solutions
- starting with 0 for all weights never changes anything
- if weights are near-zero, the operative part of the sigmoid is near-linear and such is the model
- usually chosen randomly near-zero (e.g. Xavier Glorot)
- model hence starts out as linear, and chooses direction where non-linearity is needed

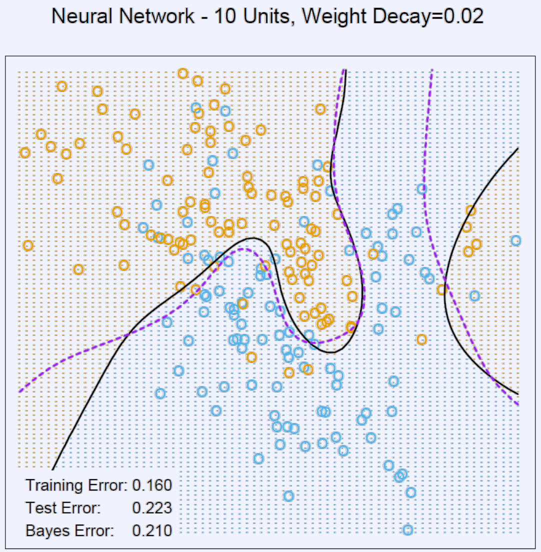
Overfitting

- early stopping amounts to shrinking the model towards a more linear solution
- weight decay is analogue to ridge regression, adds a penalty to the error
  $R(\theta) + \lambda J(\theta)$ *with* $J(\theta) = \sum_{km} \beta_{km}^2 + \sum_{ml} \alpha_{ml}^2$
- cross validation used to choose λ respectively adds $2\beta_{km}$ and $2\alpha_{ml}$ to the gradient

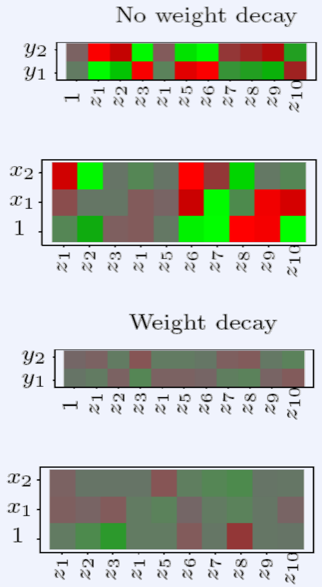
The Effect of Weight Decay



Training Error: 0.100
Test Error: 0.259
Bayes Error: 0.210



Training Error: 0.160
Test Error: 0.223
Bayes Error: 0.210



- alternative **weight elimination** penalty $J(\theta) = \sum_{km} \frac{\beta_{km}^2}{1+\beta_{km}^2} + \sum_{ml} \frac{\alpha_{ml}^2}{1+\alpha_{ml}^2}$ shrinks smaller weights more

Issues with Training

Scaling the inputs

- determines the scaling of the weights in the bottom layer(s)
- can have a large effect on the outcome

Best to normalize the inputs to mean 0 and standard deviation 1

- treats all inputs equally in regularization
- allows meaningful ranges for initial weights, e.g. uniform $[-0.7, +0.7]$

Issues with Training

Number of hidden units

- better too many than too few
- with too few, not enough flexibility for capturing the non-linear effect
- with too many, the superfluous ones can be shrunk during regularization

Typically 50 to 100 hidden units

- increasing with number of inputs and training instances
- need not use CV to find the optimal number if you use CV to tune λ
- choice guided partly by background knowledge

Modern NNs are heavily overparametrized

Issues with Training

Number of hidden layers

- allows hierarchical extraction of features at different levels of resolution
- choice guided partly by background knowledge

$R(\theta)$ potentially possesses very many minima

- thus need to try several starting configurations
- good idea to combine models by averaging their output
- bagging is another possibility (changes training data instead of starting values)

Example Sigmoids and Radials

Generate data from two additive error models

- sum of sigmoids: $Y = \sigma(a_1^T X) + \sigma(a_2^T X) + \epsilon_1$ with $a_1 = (3,3), a_2 = (3,-3)$
- radial: $Y = \prod_{m=1}^{10} \phi(X_m) + \epsilon_2$ with $\phi(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2}$
- $X = (X_1, X_2, \dots, X_p)$ with each X_i being a standard Gaussian variable
- ϵ_i are Gaussian errors, variance chosen such that S/N ratio = 4

Signal to Noise (S/N) ratio $\frac{Var(E[Y|X])}{Var(Y-E[Y|X])} = \frac{Var(f(x))}{Var(\epsilon)}$

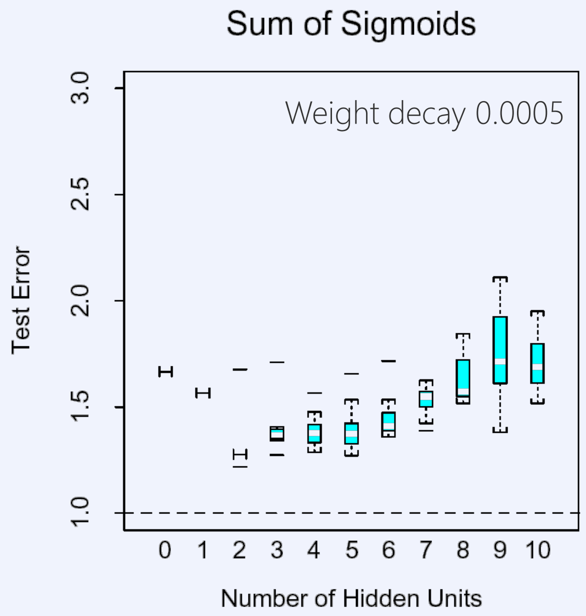
- 100 training samples and 10,000 test samples

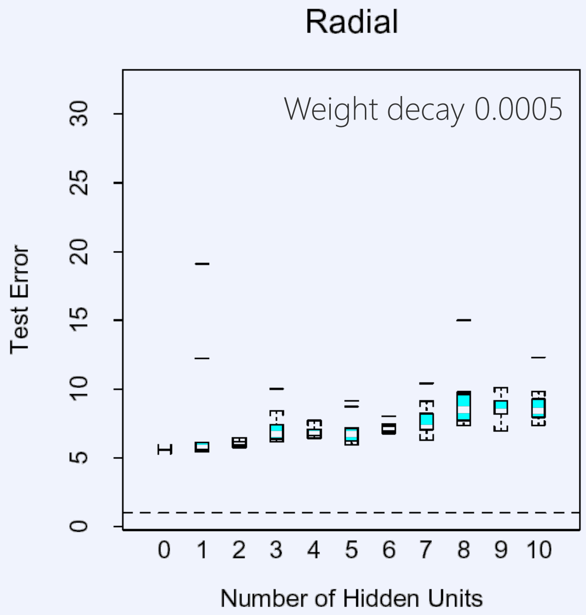
Fit neural network with weight decay $(\lambda = 0.0005)$ and various numbers of hidden units

- record average test error $E_{\text{test}}\left[Y - \hat{f}(X)\right]^2$ over 10 random initializations

Example Sigmoids and Radials

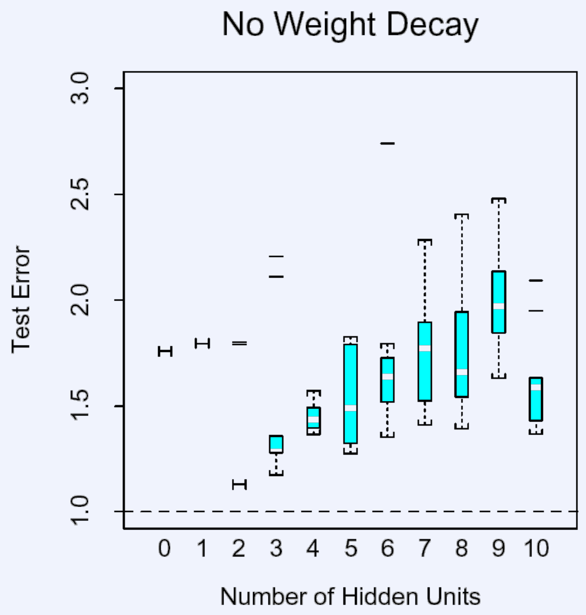
- radial is the "worst" case since no preferred directions (each hidden neuron represents a direction), and worse than the best constant model (which has relative error 5 for a S/N ratio of 4)

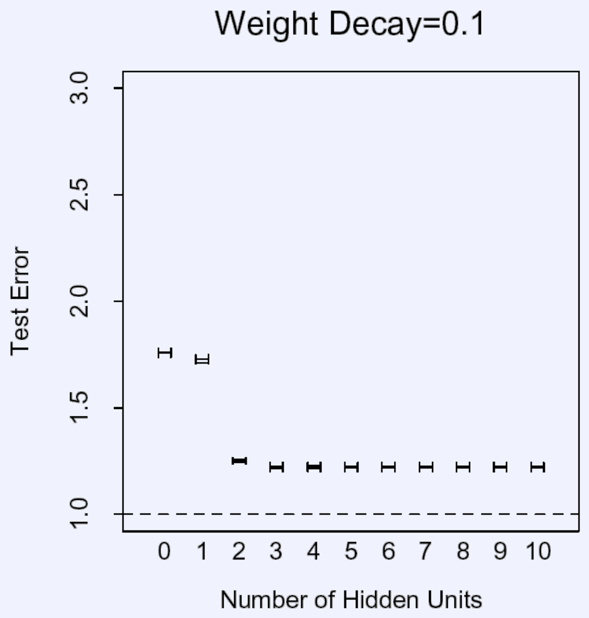




Example Sigmoids – Effect of Weight Decay

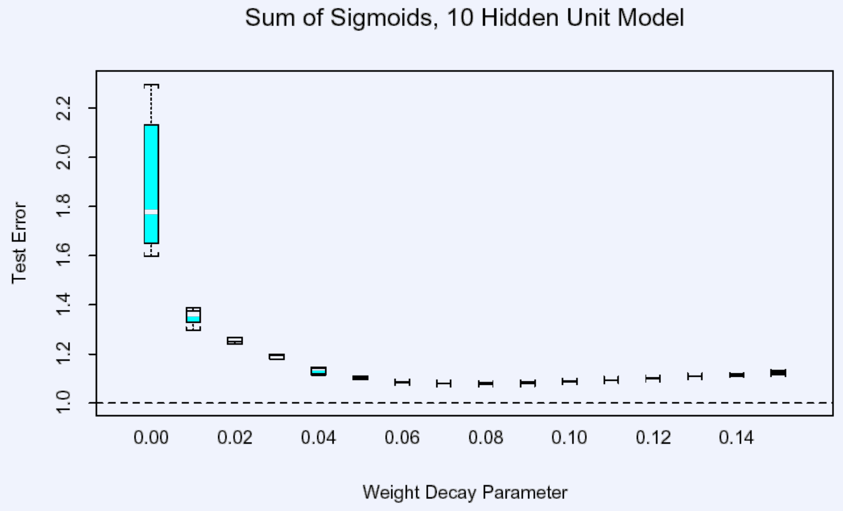
Weight decay helps to reduce the test error





Example Sigmoids – Determining λ

$\lambda = 0.1$ is about optimal



Example Sigmoids and Radials

We need to select

- the number of hidden units M
- the weight decay parameter λ

One possibility

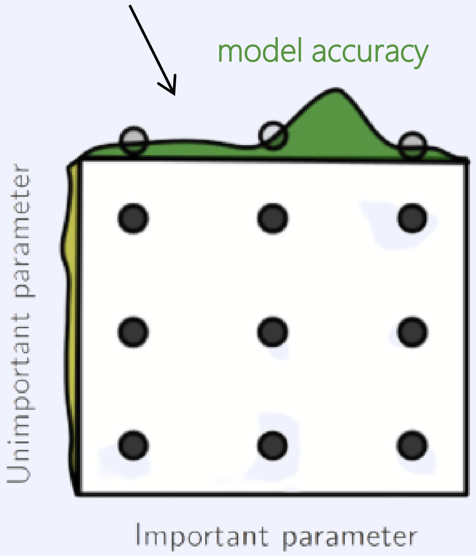
- fix either parameter at the point of the least constrained model (to allow flexibility)
- choose the other parameter with CV
- here least constrained is $\lambda = 0$, $M = 10$
- for our example optimizing λ was more effective than optimizing M

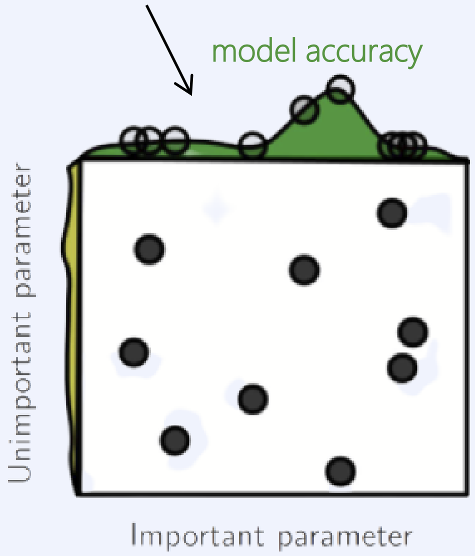
Another possibility: try different configurations of (λ, M)

Note on Hyperparameter Tuning

Another possibility: try different combinations of (λ, M)

Careful: **grid** search is usually much worse than **random** search



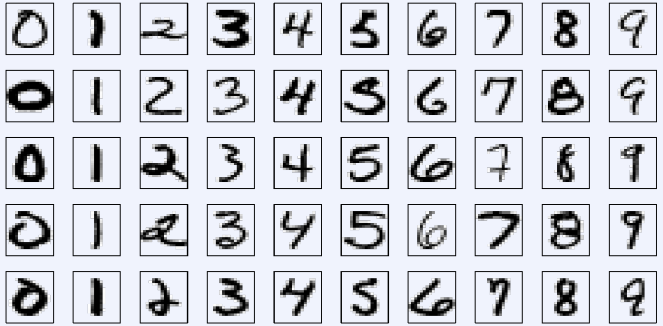


(Bergstra and Bengio, "Random Search for Hyper-Parameter Optimization")

Example Zip Code Data

Data is 16x16 8-bit grayscale images

- 256 inputs to the neural net, one per pixel
- 320 digits in training set, 160 digits in test set



A black-box neural net is not appropriate

- pixel representation lacks invariances, e.g. to small rotations
- early-day neural nets hence yielded low accuracy (4.5%)
- here we report on breakthrough effort to overcome this

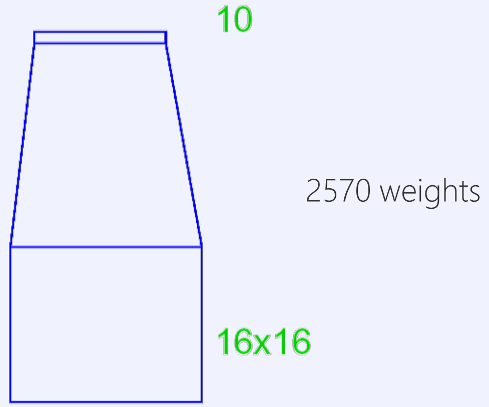
Sigmoidal output units

- fit with square error function
- online training
- training error 0% (more parameters than observations)

Example Zip Code Data

Five classification networks

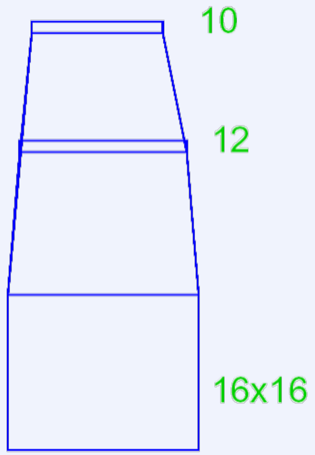
- Net-1: no hidden layers, equivalent to logistic regression



Example Zip Code Data

Five classification networks

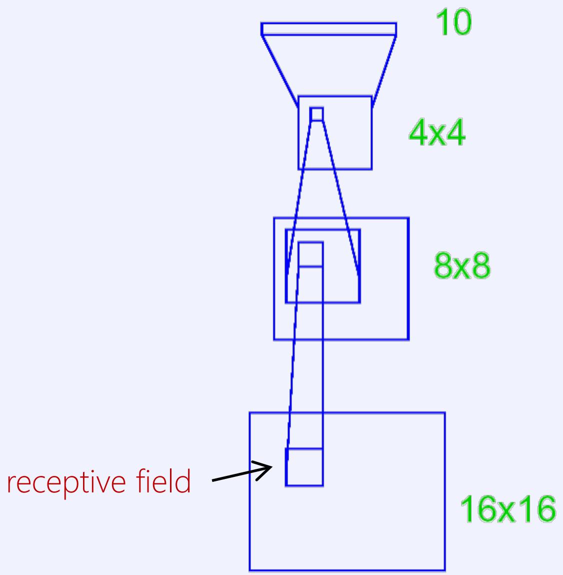
- Net-1: no hidden layers, equivalent to logistic regression
- Net-2: 1 layer, 12 units, fully connected



Example Zip Code Data

Five classification networks

- Net-1: no hidden layers, equivalent to logistic regression
- Net-2: 1 layer, 12 units, fully connected
- Net-3: 2 layers locally connected

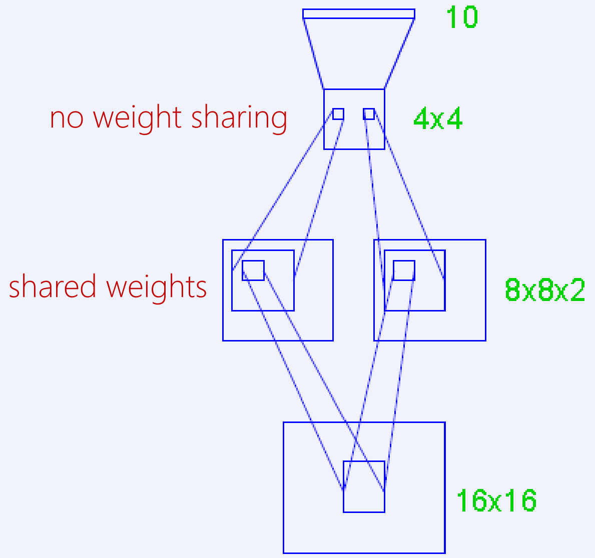


- local connectivity: receptive field of adjacent units in the first (second) hidden layer are two (one) units apart

Example Zip Code Data

Five classification networks

- Net-1: no hidden layers, equivalent to logistic regression
- Net-2: 1 layer, 12 units, fully connected
- Net-3: 2 layers locally connected
- Net-4: like Net-3 with weight sharing



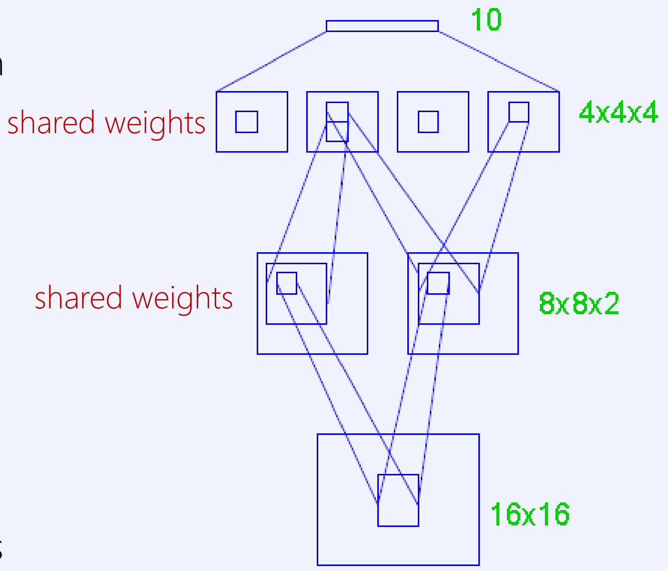
- **local connectivity**: receptive field of adjacent units in the first (second) hidden layer are two (one) units apart

- **shared weights**: same weights among all receptive fields in a feature map, but individual bias

Example Zip Code Data

Five classification networks

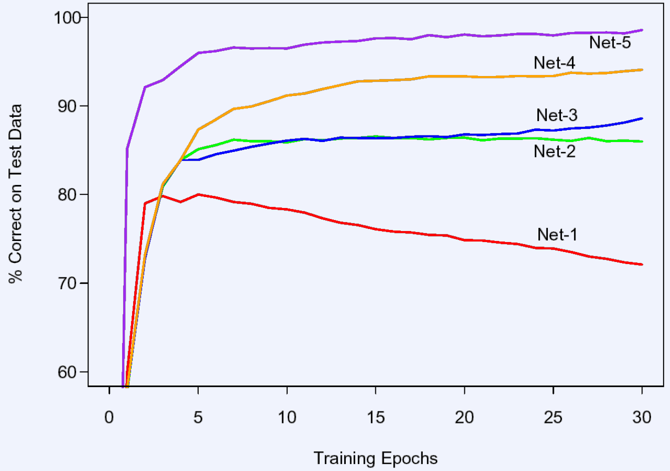
- Net-1: no hidden layers, equivalent to logistic regression
- Net-2: 1 layer, 12 units, fully connected
- Net-3: 2 layers locally connected
- Net-4: like Net-3 with weight sharing
- Net-5: like Net-4 with 2 levels of weight sharing



- **local connectivity**: receptive field of adjacent units in the first (second) hidden layer are two (one) units apart
- **shared weights**: same weights among all receptive fields in a feature map, but individual bias

Example Zip Code Data

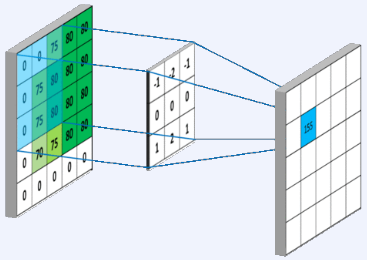
NNs are especially effective for problems with high signal-to-noise ratio & spatial redundancy
However they lack the ability to interpret the prediction

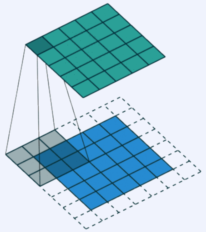


Network	Links	Weights	% Correct
Net-1	2570	2570	80.0
Net-2	3214	3214	87.0
Net-3	1226	1226	88.5
Net-4	2266	1132	94.0
Net-5	5194	1060	98.4

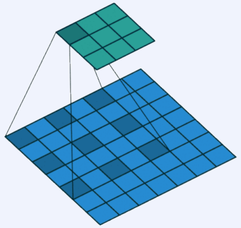
Convolutional Neural Networks

We slide a kernel/filter over the image

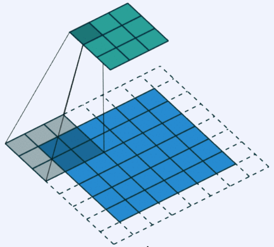




padding

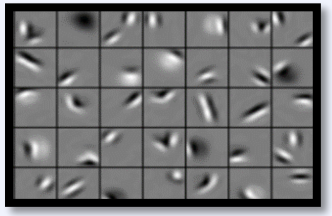


dilation

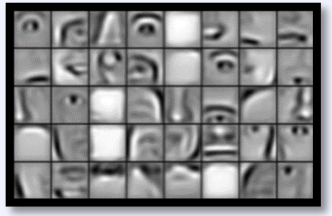


stride

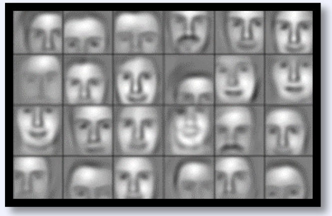
We can visualize the learned filters in each layer



layer 1 filter



layer 2 filter



layer 3 filter

Deep Learning

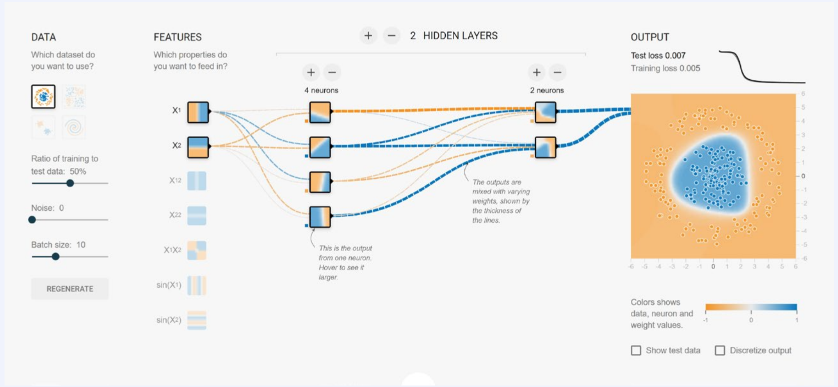
Current hype in neural networks

- build deep (multilayer) and wide networks
- layers learn a hierarchy of problem features, as exemplified by the digit example above
- adjust training schedule (some layers learn faster than others)
- results in high accuracy models
- especially suitable for image analysis and natural language problems

Very well written online textbook: Neural Networks and Deep Learning by Michael Nielsen

A Neural Network Playground

[Tinker with a NN directly in your browser] [Tinker with a CNN in your browser]



Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

Which properties do you want to feed in?

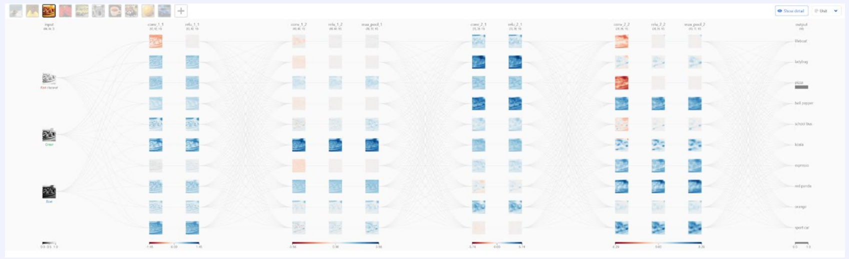
This is the output from one neuron. Hover to see it larger.

The outputs are mixed with varying weights, shown by the thickness of the lines.

Test loss 0.007
Training loss 0.005

Colors shows data, neuron and weight values.

☐ Show test data ☐ Discretize output



Summary

Neural networks automatically learn the transformation from the data

Feed-forward NN: several layers of linear transformations followed by a nonlinearity

We train NNs with gradient descent (backpropagation via automatic differentiation)

There are many hyperparameters to tune: num. neurons, num. hidden layers, weight decay

Suitable for problems with high SNR and (spatial) redundancy: images, text, audio, graphs, …