PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 5: NEURAL NETWORKS

Learning Objectives

1、What are feed-forward network functions?

2、What are cost functions for network training?

3、What are error propagation schemes for neural networks?

4、How to compute Jacobian and Hessian matrices?

5、How to achieve regularization for neural networks?

6、What are Bayesian MAP neural networks?

7、What are convolution neural networks?

8、What are generative adversarial networks?

Outlines

- Feedforward Network Functions
- Network Training
- Error Backpropagation
- Jacobian and Hessian Matrices
- Network Regularization
- MAP Neural Networks
- CNN and GAN

Feed-forward Network Functions

- Goal: to extend linear model by making the basis functions depend on parameters, allow these parameters to be adjusted.

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

First layer

activations

weights

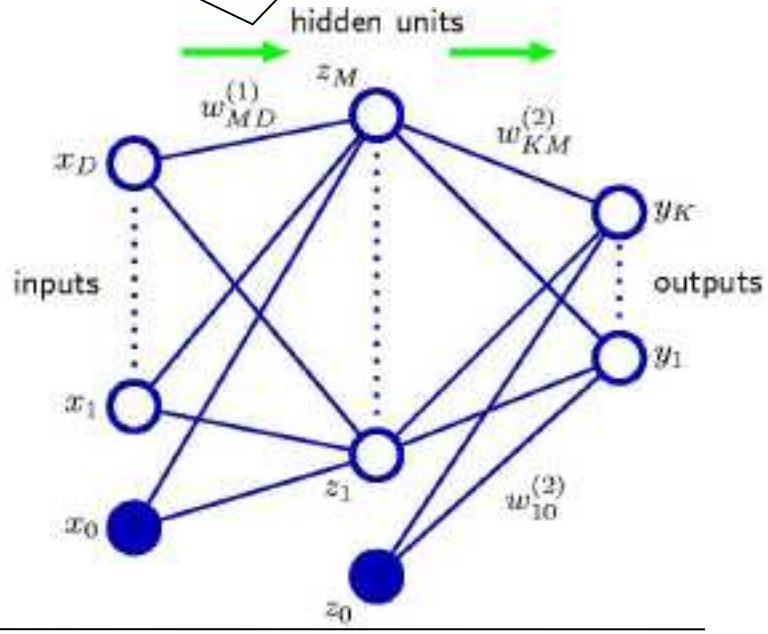
biases

Forward propagation of information

$$z_j = h(a_j)$$

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

$$y_k = \sigma(a_k)$$

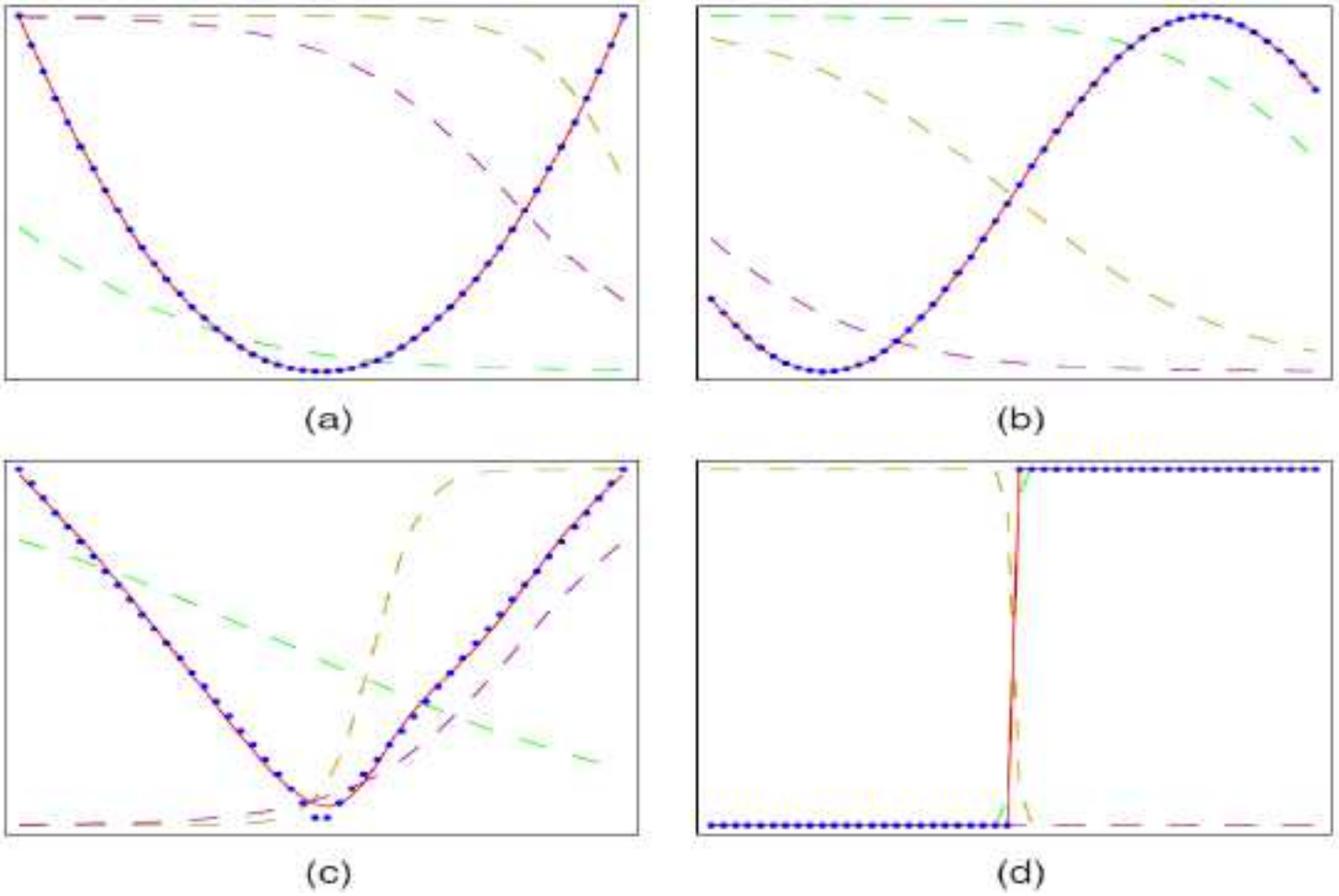


Feed-forward Network Functions

- The overall network function, comprising two stage processing, becomes a linear regression model with adaptive basis functions

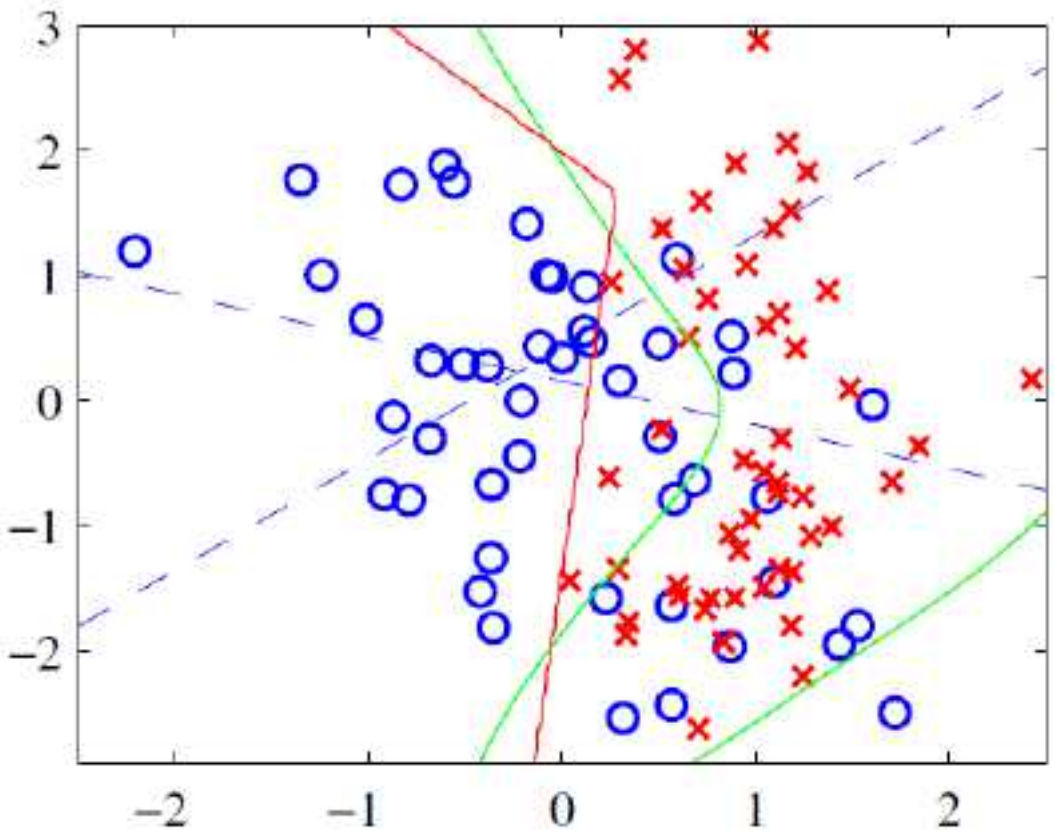
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\underbrace{\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right)}_{\text{Adaptive basis functions}} + w_{k0}^{(2)}\right)$$

Feed-forward Network Functions



The capability of network functions to approximate different functions

Feed-forward Network Functions



The capability of network functions to form the decision surface: **red line**;
the optimal decision surface: **green line**

Outlines

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Network Training (I)

- t has a Gaussian distribution with an x-dependent mean

$$p(t|\mathbf{x}, \mathbf{w}) = \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{w}, \beta) \qquad \text{(likelihood function)}$$

$$\frac{\beta}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2 - \frac{N}{2}\ln\beta + \frac{N}{2}\ln(2\pi) \qquad \text{(Negative log)}$$

Network Training (II)

- Maximizing the likelihood function is equivalent to minimizing the sum-of-squares error function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

- Having found $\mathbf{w}_{ML}$, the value of β can be found by minimizing negative log likelihood

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{y(\mathbf{x}_n, \mathbf{w}_{\mathrm{ML}}) - t_n\}^2$$

Network Training (III)

- The choice of output unit activation function and matching error function
  - ✓ Standard regression problems:

    Error function: Negative log-likelihood function

    Output unit activation function: identity

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

$$y = a$$

Network Training (IV)

- The choice of output unit activation function and matching error function
  - ✓ For binary classification problems:

    Error function: cross-entropy error function

    Output unit activation function: logistic sigmoid

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

$$y = \sigma(a) \equiv \frac{1}{1 + \exp(-a)}$$

Network Training (V)

- The choice of output unit activation function and matching error function
  - ✓ For multiclass problems:

    Error function: cross-entropy error function

    Output unit activation function: softmax function

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{kn} \ln y_k(\mathbf{x}_n, \mathbf{w})$$

$$y_k(\mathbf{x}, \mathbf{w}) = \frac{\exp(a_k(\mathbf{x}, \mathbf{w}))}{\sum_j \exp(a_j(\mathbf{x}, \mathbf{w}))}$$

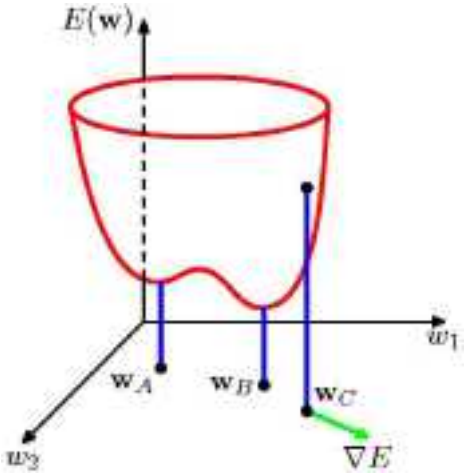
Parameter Optimization

- Error E(w) is a smooth continuous function of w and smallest value will occur at a point in weight space

$$\nabla E(\mathbf{w}) = 0$$

Global minimum: $\mathbf{w}_{\mathrm{B}}$

Local minima: $\mathbf{w}_{\mathrm{A}}$



- Most techniques involve choosing some initial value for weight vector and then moving through weight space in a succession of steps of the form

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \Delta\mathbf{w}^{(\tau)}$$

Local Quadratic Approximation

- Taylor expansion of E(w) around some point

$$E(\mathbf{w}) \simeq E(\widehat{\mathbf{w}}) + (\mathbf{w} - \widehat{\mathbf{w}})^{\mathrm{T}}\mathbf{b} + \frac{1}{2}(\mathbf{w} - \widehat{\mathbf{w}})^{\mathrm{T}}\mathbf{H}(\mathbf{w} - \widehat{\mathbf{w}})$$

$\mathbf{b} \equiv \nabla E|_{\mathbf{w}=\widehat{\mathbf{w}}}$ (gradient) $\quad (\mathbf{H})_{ij} \equiv \left.\frac{\partial E}{\partial w_i \partial w_j}\right|_{\mathbf{w}=\widehat{\mathbf{w}}}$ (Hessian Matrix)

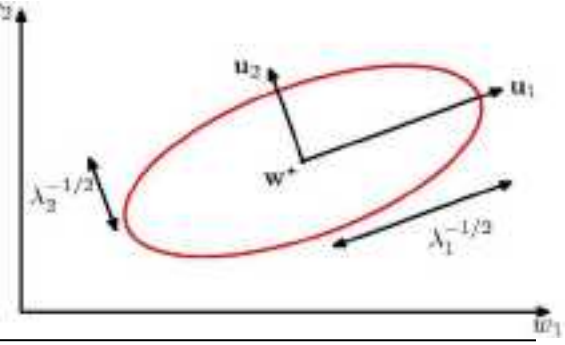
- Local approximation of the gradient

$$\nabla E \simeq \mathbf{b} + \mathbf{H}(\mathbf{w} - \widehat{\mathbf{w}}) \qquad \text{If } b = 0, \quad \widehat{\mathbf{w}} = \mathbf{w} - \mathbf{H}^{-1}\nabla E$$

- Local quadratic approximation when $b = 0$ at w*

$$E(\mathbf{w}) = E(\mathbf{w}^\star) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^\star)^{\mathrm{T}}\mathbf{H}(\mathbf{w} - \mathbf{w}^\star)$$

$$\Longrightarrow \quad E(\mathbf{w}) = E(\mathbf{w}^\star) + \frac{1}{2}\sum_i \lambda_i \alpha_i^2$$



Use of Gradient Information

- In the quadratic approximation, computational cost to find minimum is $O(W^3)$

  W is the dimensionality of w

  - ✓ perform $O(W^2)$ evaluations, each of which would require O(W) steps.

- In an algorithm that makes use of the gradient information, computational cost is $O(W^2)$

  - ✓ By using error backpropagation, O(W) gradient evaluations and each such evaluation takes only O(W) steps.

Gradient Descent Optimization

- Weight update to comprise a small step in the direction of the negative gradient

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E(\mathbf{w}^{(\tau)})$$

- Batch method
  - ✓ Techniques that use the whole data set at once.
  - ✓ The error function always decreases at each iteration unless the weight vector has arrived at a local or global minimum.

- On-line version of gradient descent
  - ✓ Sequential gradient descent or stochastic gradient descent
  - ✓ Update to the weight vector based on one data point at a time.
  - ✓ Can handle redundancy in the data much more efficiently.
  - ✓ The possibility of escaping from local minima.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)})$$

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Error Backpropagation (I)

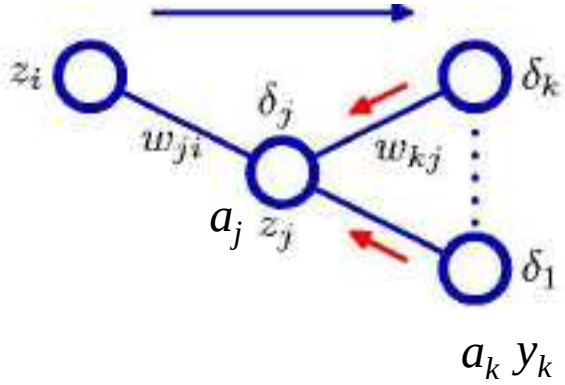
- Least Square Error Function

$$E = \sum_n E_n \qquad E_n = \frac{1}{2}\sum_k (y_k - t_k)^2$$

$$y_k = a_k \qquad \frac{\partial y_k}{\partial a_k} = 1$$

$$\frac{\partial E_n}{\partial y_k} = \frac{\partial E_n}{\partial a_k} = y_k - t_k$$

Error Backpropagation (II)



$$a_j = \sum_i w_{ji} z_i \qquad z_j = h(a_j) \qquad \frac{\partial a_j}{\partial w_{ji}} = z_i$$

$$a_k = \sum_j w_{kj} z_j \qquad y_k = a_k \qquad \delta_j \equiv \frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial a_j}$$

$$\delta_k \equiv \frac{\partial E_n}{\partial a_k} = y_k - t_k \qquad \delta_j = h'(a_j) \sum_k w_{kj} \delta_k$$

$$\frac{\partial E_n}{\partial w_{kj}} = \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}} = \delta_k z_j$$

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} = \delta_j z_i$$

δ rules

Error Backpropagation (III)

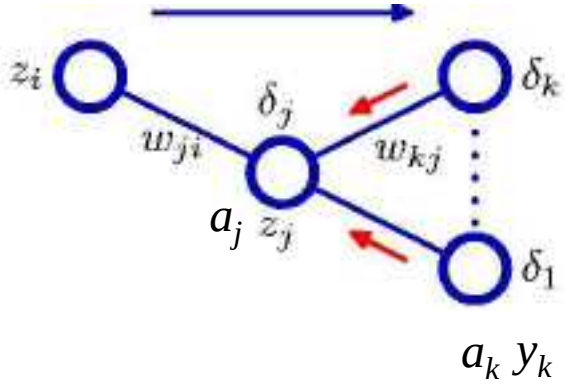
- Cross-Entropy Error Function

$$E = \sum_n E_n \qquad E_n = -\sum_k t_k \ln y_k + (1 - t_k)\ln(1 - y_k)$$

$$\frac{\partial E_n}{\partial y_k} = -\frac{t_k}{y_k} + \frac{1 - t_k}{1 - y_k} = \frac{y_k - t_k}{y_k(1 - y_k)}$$

$$\frac{\partial y_k}{\partial a_k} = y_k(1 - y_k) \qquad y_k = \sigma(a_k)$$

Error Backpropagation (IV)



$$a_j = \sum_i w_{ji} z_i \qquad z_j = h(a_j) \qquad \frac{\partial a_j}{\partial w_{ji}} = z_i$$

$$a_k = \sum_j w_{kj} z_j \qquad y_k = \sigma(a_k) \qquad \delta_j \equiv \frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial a_j}$$

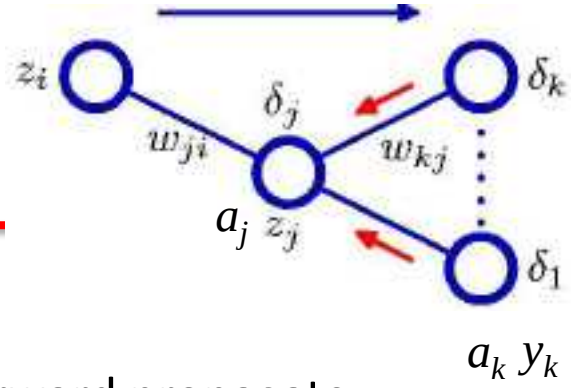
$$\delta_k \equiv \frac{\partial E_n}{\partial a_k} = y_k - t_k \qquad \delta_j = h'(a_j) \sum_k w_{kj} \delta_k$$

$$\frac{\partial E_n}{\partial w_{kj}} = \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}} = \delta_k z_j$$

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} = \delta_j z_i$$

δ rules

Error Backpropagation (V)



Error Backpropagation

① Apply an input vector x_n to the network and forward propagate through the network using equations below to find the activations of all the hidden and output units.

$$a_j = \sum_i w_{ji} z_i \qquad z_j = h(a_j)$$

② Evaluate the δ_k for all the output units using $\delta_k = y_k - t_k$

③ Backpropagate the δ using $\delta_j = h'(a_j) \sum_k w_{jk} \delta_k$

to obtain δ_j for each hidden unit in the network

④ Use $\dfrac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$ to evaluate the required derivatives

A Simple Example

$$h(a) \equiv \tanh(a)$$

$$\tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$

$$h'(a) = 1 - h(a)^2$$

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(y_k - t_k)^2$$

(y_k: output unit k, t_k: the corresponding target)

$$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i$$

$$z_j = \tanh(a_j)$$

$$y_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j$$

$$\delta_j = (1 - z_j^2)\sum_{k=1}^{K} w_{kj}\delta_k$$

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i \qquad \frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

δ rules

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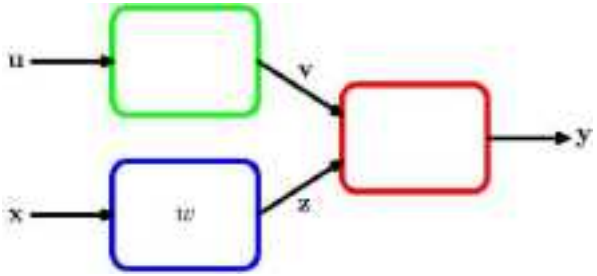
The Jacobian Matrix

- The technique of backpropagation can also be applied to the calculation of other derivatives.
- The Jacobian matrix
  - ✓ Elements are given by the derivatives of the network outputs w.r.t. the inputs

$$J_{ki} \equiv \frac{\partial y_k}{\partial x_i}$$



  - ✓ Minimizing an error function *E* w.r.t. the parameter w

$$\frac{\partial E}{\partial w} = \sum_{k,j} \frac{\partial E}{\partial y_k} \frac{\partial y_k}{\partial z_j} \frac{\partial z_j}{\partial w}$$

The Jacobian Matrix

- A measure of the *local sensitivity* of the outputs to change in each of the input variables.
  - ✓ In general, the network mapping is nonlinear, and so the elements will not be constants. This is valid provided the $|\Delta x_i|$ are small.

$$\Delta y_k \simeq \sum_i \frac{\partial y_k}{\partial x_i} \Delta x_i$$

  - ✓ The evaluation of the Jacobian Matrix

$$J_{ki} = \frac{\partial y_k}{\partial x_i} = \sum_j \frac{\partial y_k}{\partial a_j} \frac{\partial a_j}{\partial x_i} = \sum_j w_{ji} \frac{\partial y_k}{\partial a_j}$$

$$\frac{\partial y_k}{\partial a_j} = \sum_l \frac{\partial y_k}{\partial a_l} \frac{\partial a_l}{\partial a_j} = h'(a_j) \sum_l w_{lj} \frac{\partial y_k}{\partial a_l}$$

(Sigmoidal activation function)

The Hessian Matrix

- The Hessian matrix
  - ✓ The second derivatives form the elements of H, $\frac{\partial^2 E}{\partial w_{ji} \partial w_{lk}}$
  - ✓ Important roles:
    - Considering the second-order properties of the error surfaces.
    - Forms the basis of a fast procedure for re-training a feed-forward network following a small change in the training data
    - The inverse of the Hessian is used to identify the least significant weights in a network (pruning algorithm)
    - In the Laplace approximation for a Bayesian NN
  - ✓ Various approximation schemes are used to evaluate the Hessian matrix for a NN.

Hessian: Diagonal Approximation

- Inverse of the Hessian is useful, and inverse of diagonal matrix is trivial to evaluate.
- Consider an error function
  - ✓ Replaces the off-diagonal elements with zeros
  - ✓ The diagonal elements of the Hessian:

$$\frac{\partial^2 E_n}{\partial w_{ji}^2} = \frac{\partial^2 E_n}{\partial a_j^2} z_i^2$$

$$\frac{\partial^2 E_n}{\partial a_j^2} = h'(a_j)^2 \sum_k \sum_{k'} w_{kj} w_{k'j} \frac{\partial^2 E_n}{\partial a_k \partial a_{k'}} + h''(a_j) \sum_k w_{kj} \frac{\partial E^n}{\partial a_k}$$

$$\frac{\partial^2 E_n}{\partial a_j^2} = h'(a_j)^2 \sum_k w_{kj}^2 \frac{\partial^2 E_n}{\partial a_k^2} + h''(a_j) \sum_k w_{kj} \frac{\partial E_n}{\partial a_k}$$ (neglect off-diagonal)

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

Outer Product Approximation

$$\mathbf{H} = \nabla\nabla E = \sum_{n=1}^{N} \nabla y_n \nabla y_n + \sum_{n=1}^{N} (y_n - t_n)\nabla\nabla y_n$$

- Output *y* happen to be very close to the target values t, the second term will be small and can be neglected.
  - Or the value of $y - t$ is uncorrelated with the value of the second derivative term, then the whole term will average to zero.

$$\mathbf{H} \simeq \sum_{n=1}^{N} \mathbf{b}_n \mathbf{b}_n^{\mathrm{T}} \qquad \mathbf{b}_n = \nabla y_n = \nabla a_n$$

Inverse Hessian

- A procedure for approximating the inverse of the Hessian
  - ✓ First, we write the outer-product approximation
  - ✓ Derive a sequential procedure for building up the Hessian by including data points one at a time.

$$\mathbf{H}_{L+1} = \mathbf{H}_L + \mathbf{b}_{L+1}\mathbf{b}_{L+1}^{\mathrm{T}}$$

$$\mathbf{H}_{L+1}^{-1} = \mathbf{H}_L^{-1} - \frac{\mathbf{H}_L^{-1}\mathbf{b}_{L+1}\mathbf{b}_{L+1}^{\mathrm{T}}\mathbf{H}_L^{-1}}{1 + \mathbf{b}_{L+1}^{\mathrm{T}}\mathbf{H}_L^{-1}\mathbf{b}_{L+1}}$$

  - ✓ The initial matrix $H_0 = H + \alpha I$

    α is a small quantity, not sensitive to the precise value of α.

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Neural Network Regularization (I)

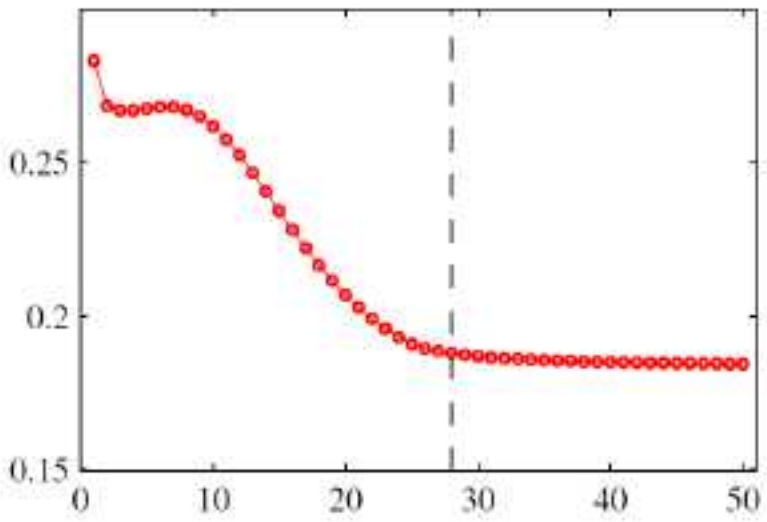
- Consistent Gaussian prior

$$p(\mathbf{w}) \propto \exp\left(-\frac{1}{2}\sum_{k}\alpha_k\|\mathbf{w}\|_k^2\right)$$

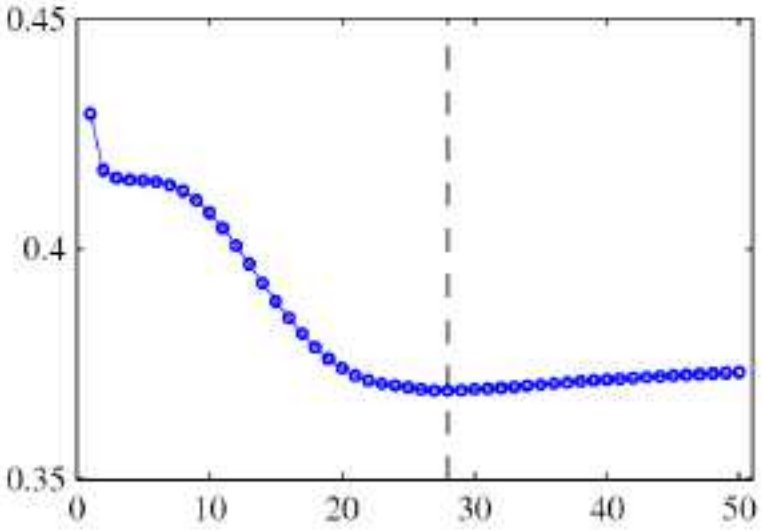
$$\|\mathbf{w}\|_k^2 = \sum_{j\in\mathcal{W}_k} w_j^2.$$

Neural Network Regularization (II)

- Early stopping



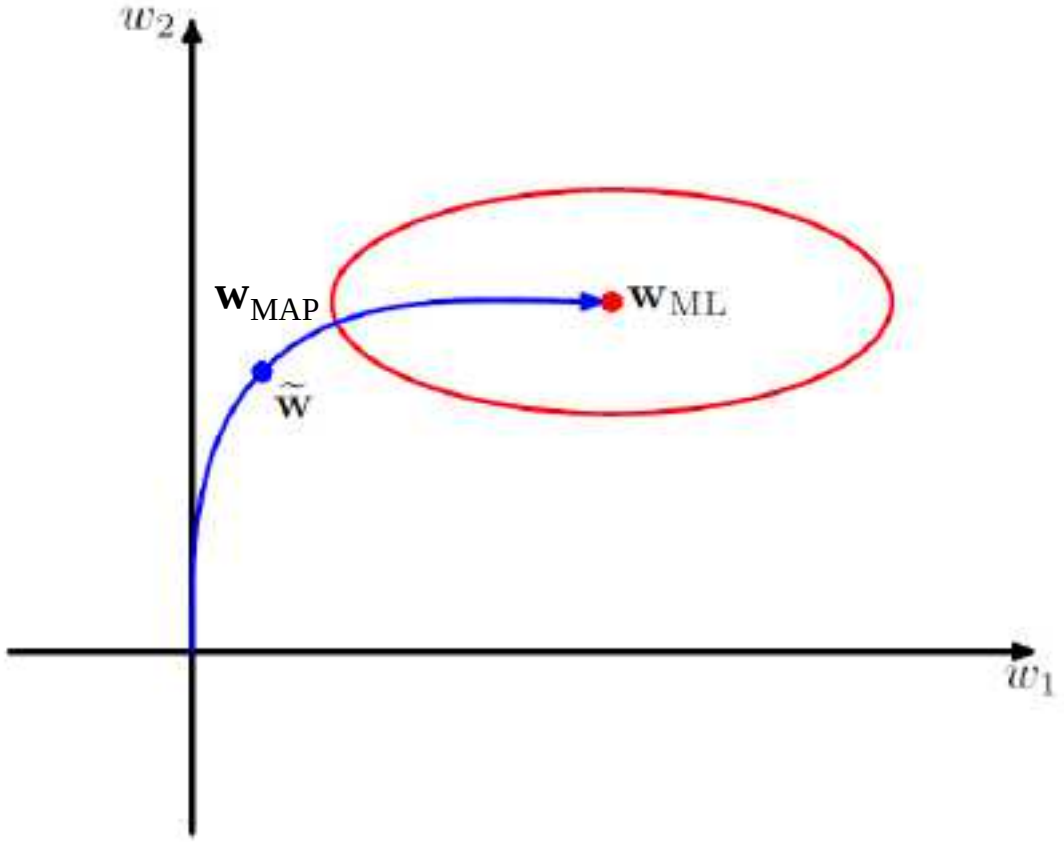
Training Error



Validation Error

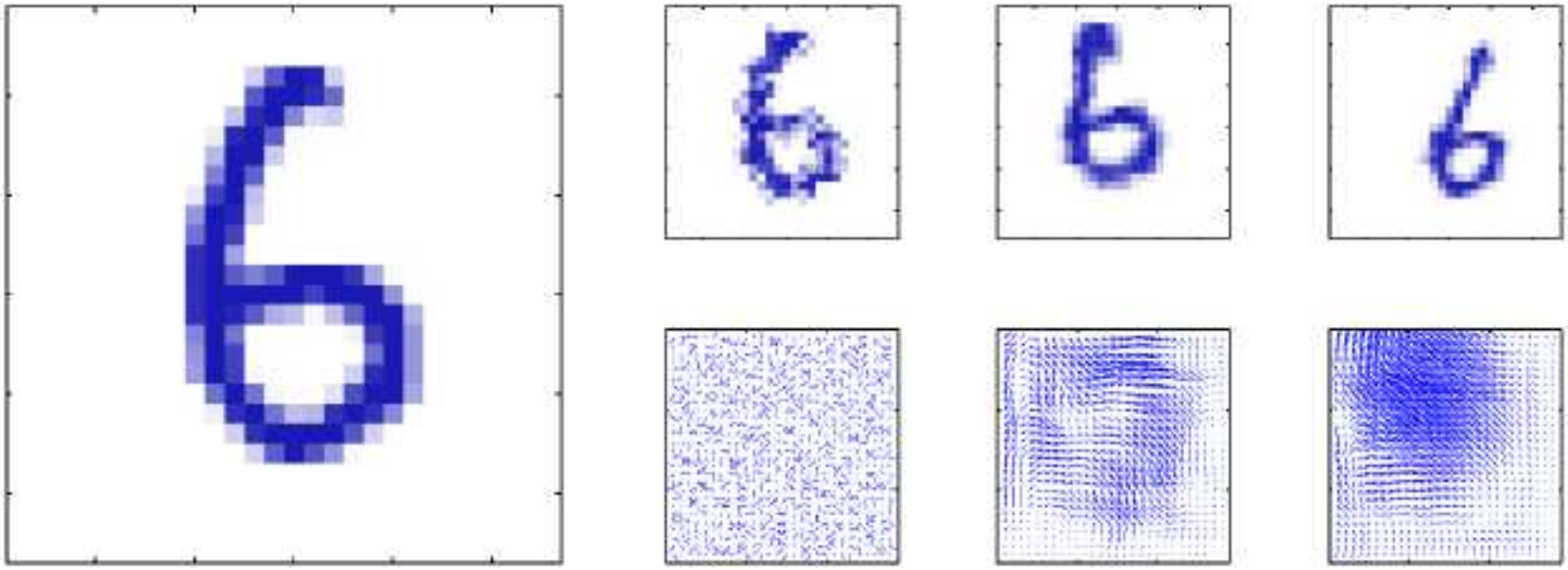
Neural Network Regularization (II)

- Early stopping



Neural Network Regularization (III)

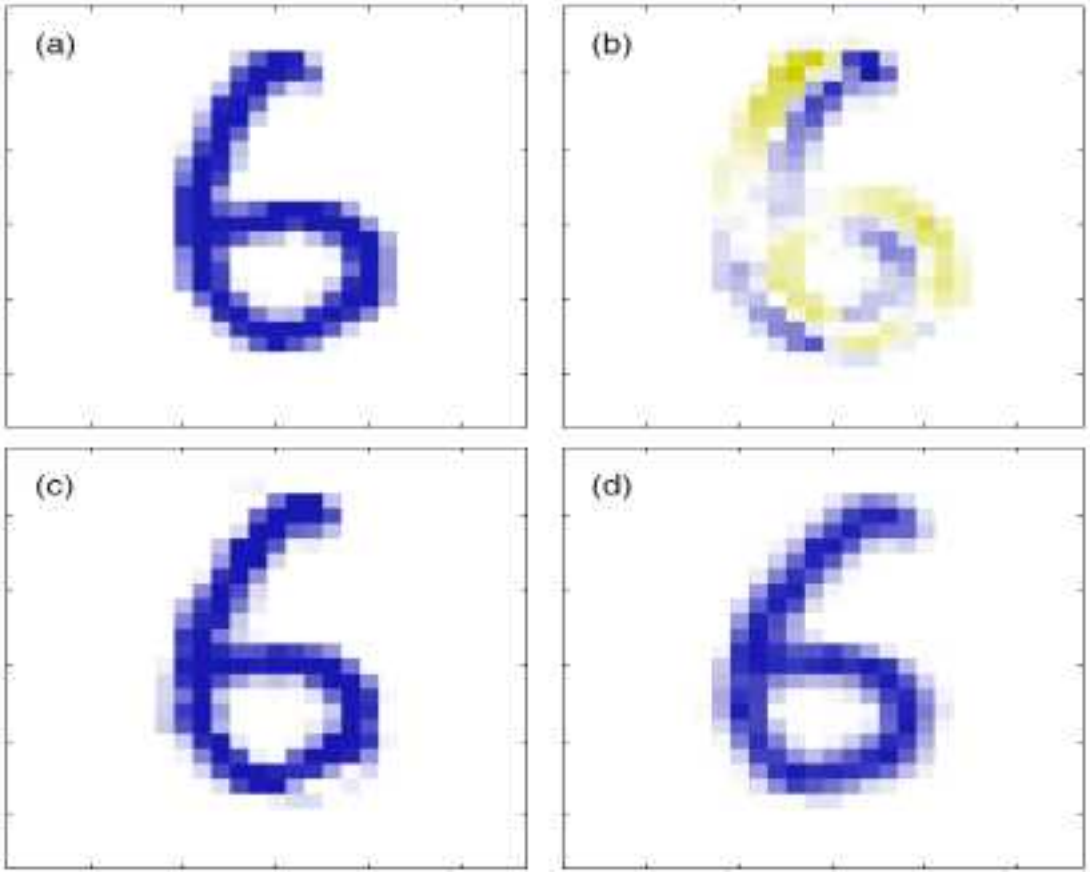
- Invariances



Data Augmentation with random displacement fields and Gaussian smoothing

Neural Network Regularization (IV)

- Tangent propagation



Data Augmentation

Neural Network Regularization (V)

- Training with transformed data

$$E = \frac{1}{2} \iint \{y(\mathbf{x}) - t\}^2 p(t|\mathbf{x}) p(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$

$$\widetilde{E} = \frac{1}{2} \iiint \{y(\mathbf{s}(\mathbf{x}, \xi)) - t\}^2 p(t|\mathbf{x}) p(\mathbf{x}) p(\xi) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \, \mathrm{d}\xi$$

$$\begin{aligned}
\widetilde{E} &= \frac{1}{2} \iint \{y(\mathbf{x}) - t\}^2 p(t|\mathbf{x}) p(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \\
&+ \mathbb{E}[\xi] \iint \{y(\mathbf{x}) - t\} \boldsymbol{\tau}^{\mathrm{T}} \nabla y(\mathbf{x}) p(t|\mathbf{x}) p(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \\
&+ \mathbb{E}[\xi^2] \iint \left[\{y(\mathbf{x}) - t\} \frac{1}{2} \left\{ (\boldsymbol{\tau}')^{\mathrm{T}} \nabla y(\mathbf{x}) + \boldsymbol{\tau}^{\mathrm{T}} \nabla \nabla y(\mathbf{x}) \boldsymbol{\tau} \right\} \right. \\
&\quad \left. + \left(\boldsymbol{\tau}^{\mathrm{T}} \nabla y(\mathbf{x}) \right)^2 \right] p(t|\mathbf{x}) p(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + O(\xi^3).
\end{aligned}$$

Neural Network Regularization (V)

- Training with transformed data

$$\widetilde{E} = E + \lambda\Omega$$

$$\Omega = \int \left[\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\} \frac{1}{2} \left\{ (\boldsymbol{\tau}')^{\mathrm{T}} \nabla y(\mathbf{x}) + \boldsymbol{\tau}^{\mathrm{T}} \nabla\nabla y(\mathbf{x}) \boldsymbol{\tau} \right\} + \left(\boldsymbol{\tau}^T \nabla y(\mathbf{x}) \right)^2 \right] p(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

$$\Omega = \frac{1}{2} \int \left(\boldsymbol{\tau}^T \nabla y(\mathbf{x}) \right)^2 p(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

Tangent propagation regularization

$$\Omega = \frac{1}{2} \int \left\| \nabla y(\mathbf{x}) \right\|^2 p(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

Tikhonov regularization
additional noise

Neural Network Regularization (VI)

- Soft weight sharing

$$p(\mathbf{w}) = \prod_i p(w_i) \qquad p(w_i) = \sum_{j=1}^{M} \pi_j \mathcal{N}(w_i|\mu_j, \sigma_j^2)$$

$$\Omega(\mathbf{w}) = -\sum_i \ln \left(\sum_{j=1}^{M} \pi_j \mathcal{N}(w_i|\mu_j, \sigma_j^2) \right)$$

$$\widetilde{E}(\mathbf{w}) = E(\mathbf{w}) + \lambda \Omega(\mathbf{w})$$

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- Feedforward Network Functions
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- Jacobian Matrix
- Hessian Matrix
- Regularization
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- CNN and GAN

MAP Neural Networks for Regression I

$$p(t|\boldsymbol{x},\boldsymbol{w},\beta) = N(t|y(\boldsymbol{x},\boldsymbol{w}),\beta^{-1}) \qquad p(\boldsymbol{w}) = N(\boldsymbol{w}|0,\alpha^{-1}I) \qquad p(\boldsymbol{w}|t) \propto p(\boldsymbol{w})p(t|\boldsymbol{x},\boldsymbol{w},\beta)$$

$$E(\boldsymbol{w}) = -\ln p(\boldsymbol{w}|\boldsymbol{t}) = \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + \frac{\beta}{2}\sum_{n=1}^{N}[y(\boldsymbol{x}_n,\boldsymbol{w}) - t_n]^2 + Constant$$

$$\nabla E(\boldsymbol{w}) = \alpha\boldsymbol{w} + \beta\sum_{n=1}^{N}(y_n - t_n)\boldsymbol{g}_n \qquad \boldsymbol{g} = \nabla_{\boldsymbol{w}} y(\boldsymbol{x},\boldsymbol{w})$$

$\boldsymbol{A} = \nabla\nabla E(\boldsymbol{w}) = \alpha\mathbf{I} + \beta\boldsymbol{H}$ $\qquad$ $\boldsymbol{H}$: Hessian matrix of the sum-of-error function

$$\boldsymbol{w}_{\mathrm{MAP}} \longleftarrow \boldsymbol{w}^{new} = \boldsymbol{w}^{old} - \boldsymbol{A}^{-1}\nabla E(\boldsymbol{w}) \qquad q(\boldsymbol{w}) = N(\boldsymbol{w}|\boldsymbol{w}_{MAP},\boldsymbol{A}^{-1})$$

MAP Neural Networks for Regression II

$$\mathrm{y}(\boldsymbol{x}, \boldsymbol{w}) \simeq y(\boldsymbol{x}, \boldsymbol{w}_{MAP}) + \boldsymbol{g}^{T}{}_{MAP}(\boldsymbol{w} - \boldsymbol{w}_{MAP})$$

$$p(t|\boldsymbol{x}, \boldsymbol{w}, \beta) = N(t|y(\boldsymbol{x}, \boldsymbol{w}_{MAP}) + \boldsymbol{g}^{T}{}_{MAP}(\boldsymbol{w} - \boldsymbol{w}_{MAP}), \beta^{-1})$$

$$q(\boldsymbol{w}) = N(\boldsymbol{w}|\boldsymbol{w}_{MAP}, \boldsymbol{A}^{-1})$$

$$p(t|\boldsymbol{x}, D, \alpha, \beta) = \int p(t|\boldsymbol{x}, \boldsymbol{w}, \beta) q(\boldsymbol{w}) d\boldsymbol{w}$$

$$p(t|\boldsymbol{x}, D, \alpha, \beta) = N(t|y(\boldsymbol{x}, \boldsymbol{w}_{MAP}), \boldsymbol{g}^{T}{}_{MAP}\boldsymbol{A}^{-1}\boldsymbol{g}_{MAP} + \beta^{-1})$$

Hyper-parameter Optimization

$$\alpha = \frac{\gamma}{\mathbf{w}_{\mathrm{MAP}}^{\mathrm{T}}\mathbf{w}_{\mathrm{MAP}}}$$

$$\beta\mathbf{H}\mathbf{u}_i = \lambda_i\mathbf{u}_i$$

$$\gamma = \sum_{i=1}^{W}\frac{\lambda_i}{\alpha+\lambda_i}$$

$$\frac{1}{\beta} = \frac{1}{N-\gamma}\sum_{n=1}^{N}\{y(\mathbf{x}_n,\mathbf{w}_{\mathrm{MAP}}) - t_n\}^2$$

MAP Neural Networks for Classification I

$p(\boldsymbol{w}) = N(\boldsymbol{w}|0, \alpha^{-1}I)$ $p(\boldsymbol{w}|t) \propto p(\boldsymbol{w})p(t|\boldsymbol{w})$

$$E(w) = -\ln p(w|t) = \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} - \sum_{n=1}^{N}[t_n \ln y_n + (1 - t_n)\ln(1 - y_n)]$$

$$\nabla E(w) = \alpha\boldsymbol{w} + \sum_{n=1}^{N}(y_n - t_n)\boldsymbol{g}_n$$

$\boldsymbol{A} = \nabla\nabla E(\boldsymbol{w}) = \alpha\boldsymbol{I}+\boldsymbol{H}$ $\boldsymbol{H}$: Hessian matrix of the cross-entropy function

$\boldsymbol{w}_{\mathrm{MAP}} \longleftarrow \boldsymbol{w}^{new} = \boldsymbol{w}^{old} - \boldsymbol{A}^{-1}\nabla E(\boldsymbol{w})$ $q(\boldsymbol{w}) = N(\boldsymbol{w}|\boldsymbol{w}_{MAP}, A^{-1})$

MAP Neural Networks for Classification II

$$p(t|\mathbf{x}, \mathcal{D}) = \int p(t|\mathbf{x}, \mathbf{w}) q(\mathbf{w}|\mathcal{D}) \, \mathrm{d}\mathbf{w}$$

$$p(t|\mathbf{x}, \mathcal{D}) \simeq p(t|\mathbf{x}, \mathbf{w}_{\mathrm{MAP}})$$

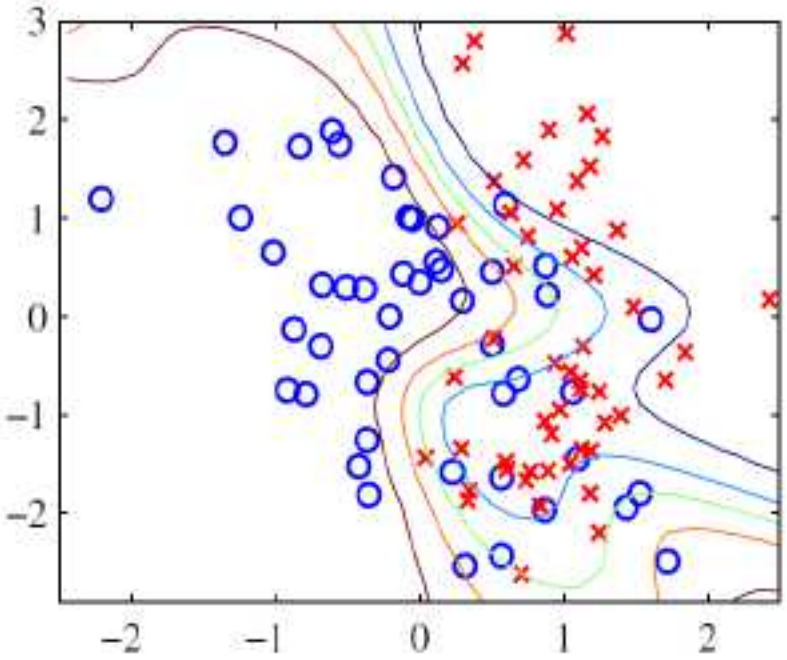
$$a(\mathbf{x}, \mathbf{w}) \simeq a_{\mathrm{MAP}}(\mathbf{x}) + \mathbf{b}^{\mathrm{T}}(\mathbf{w} - \mathbf{w}_{\mathrm{MAP}})$$

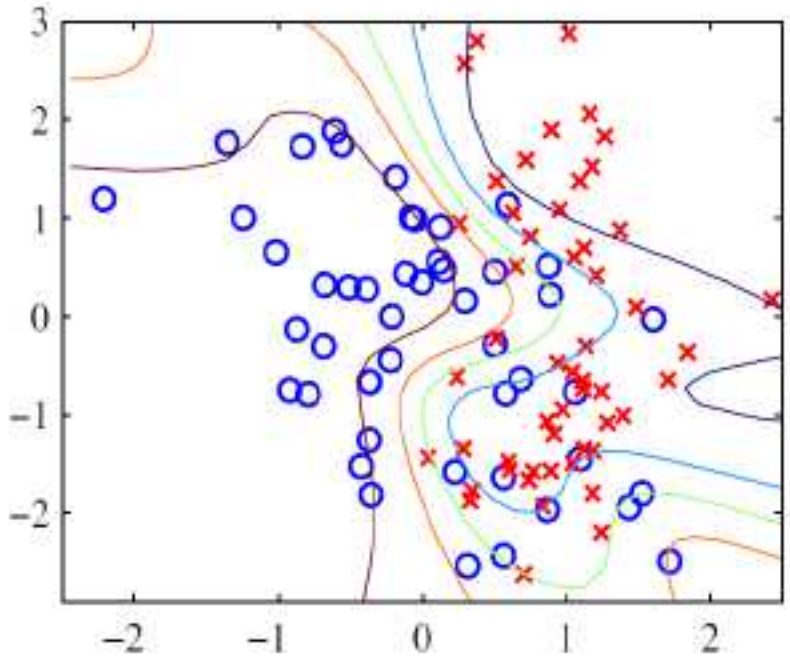
$$a_{\mathrm{MAP}}(\mathbf{x}) = a(\mathbf{x}, \mathbf{w}_{\mathrm{MAP}}) \quad \mathbf{b} \equiv \nabla a(\mathbf{x}, \mathbf{w}_{\mathrm{MAP}})$$

$$a_{\mathrm{MAP}} \equiv a(\mathbf{x}, \mathbf{w}_{\mathrm{MAP}})$$

$$\sigma_a^2(\mathbf{x}) = \mathbf{b}^{\mathrm{T}}(\mathbf{x}) \mathbf{A}^{-1} \mathbf{b}(\mathbf{x})$$

MAP Neural Networks for Classification II





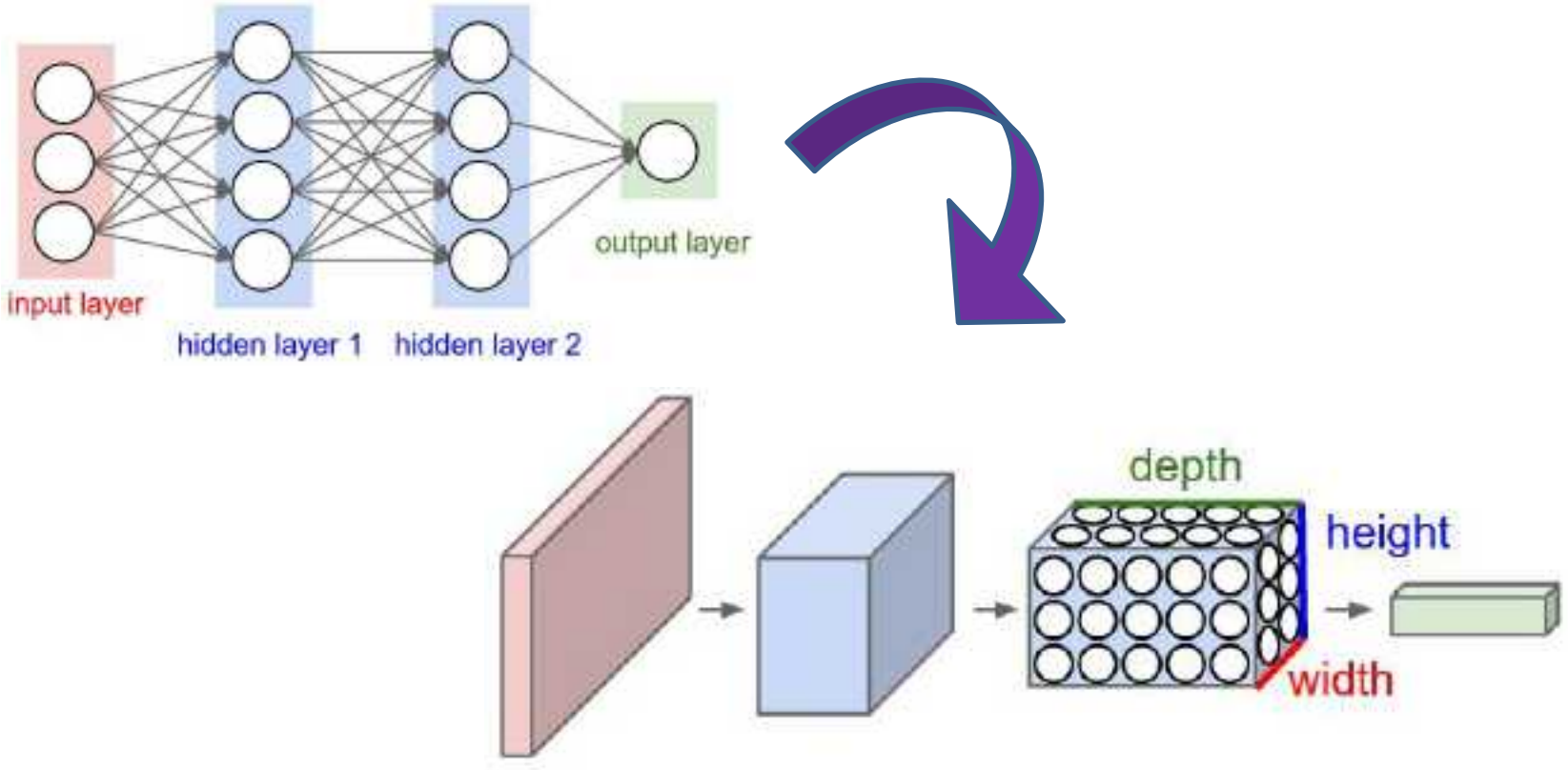
Decision boundary using MAP neural networks

Outlines

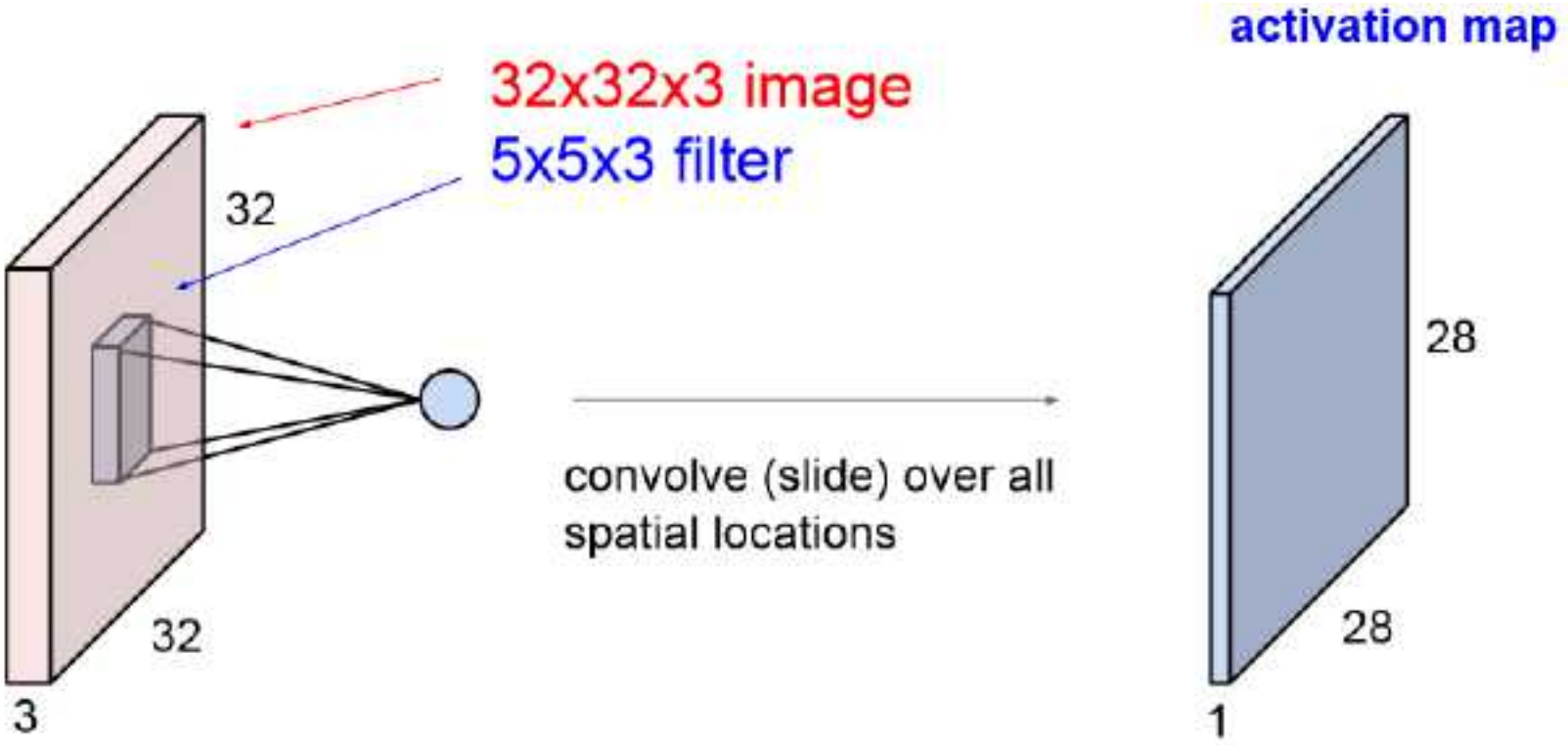
- Feedforward Network Functions
- Network Training
- Error Backpropagation
- Jacobian and Hessian Matrices
- Network Regularization
- MAP Neural Networks
- CNN and GAN

CNN Architectures

What's the same and difference between a normal full-connected network and convolution network



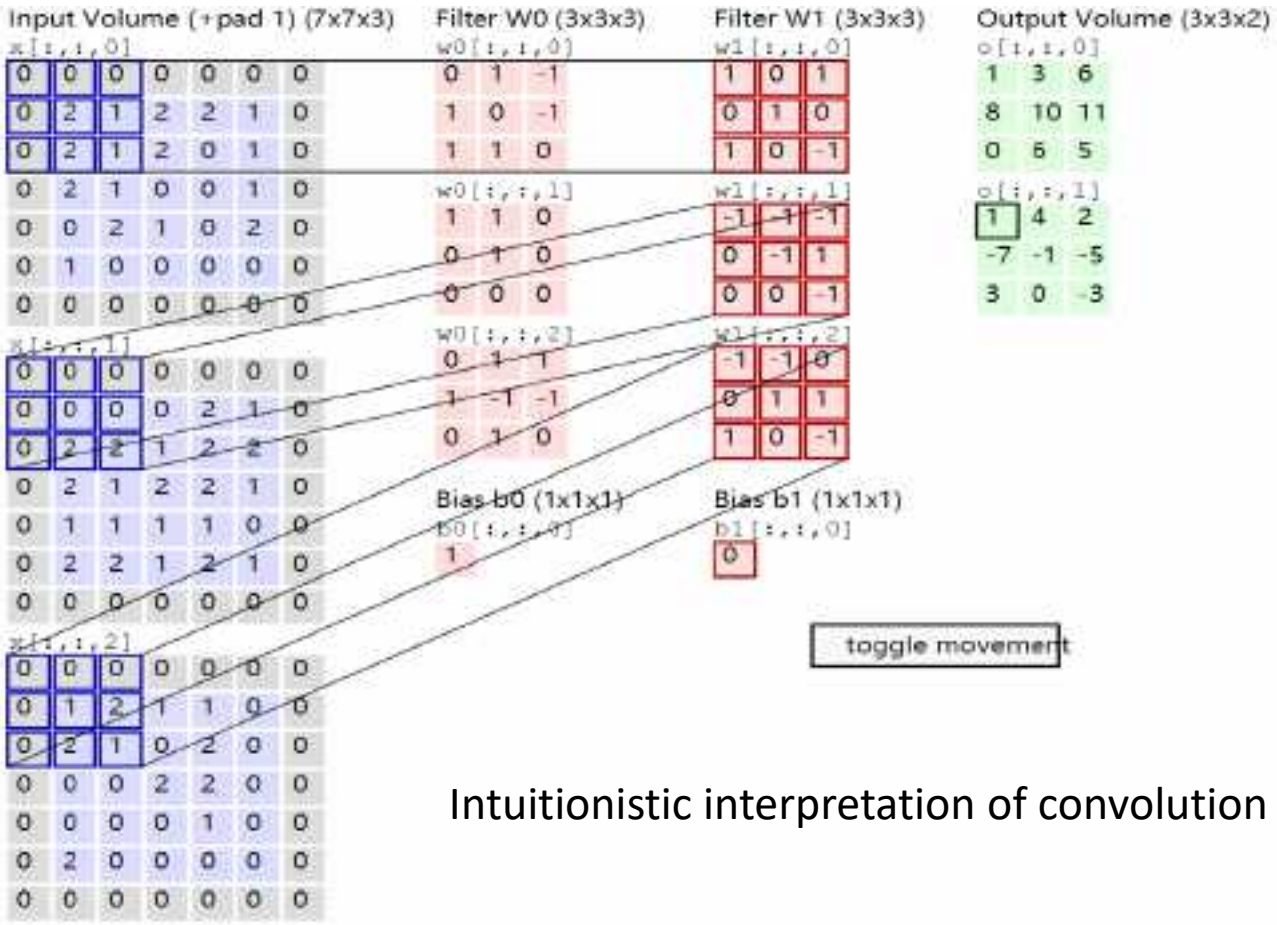
Convolution Layer



CNN Architectures

- Convolution layer
- Pooling layer
- Rectified Linear Units (ReLu) layer
- Full-connected layer

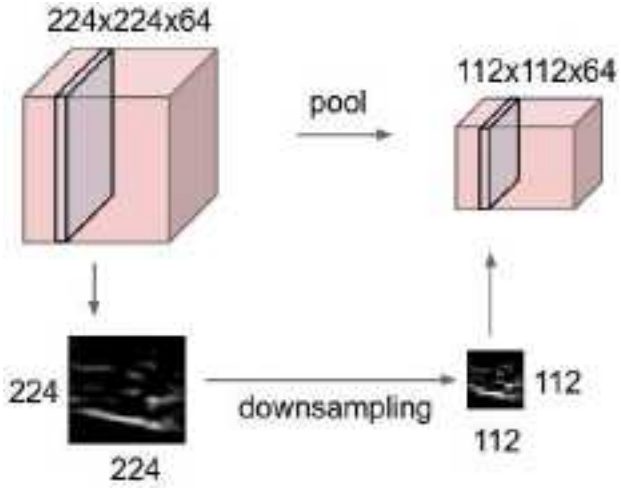
Convolution Layer

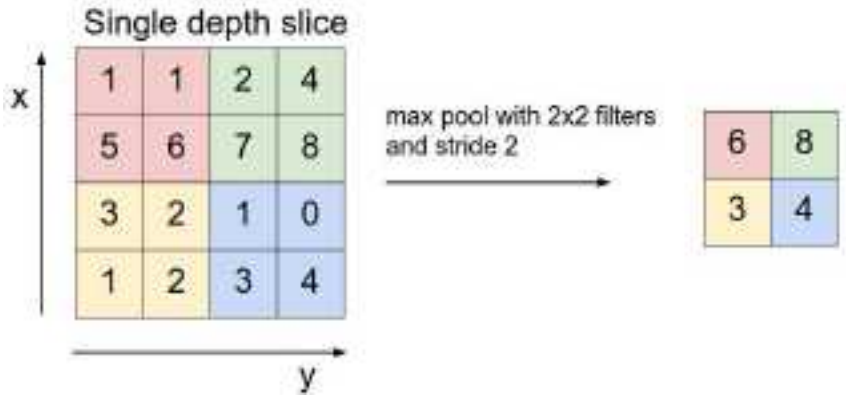


Intuitionistic interpretation of convolution

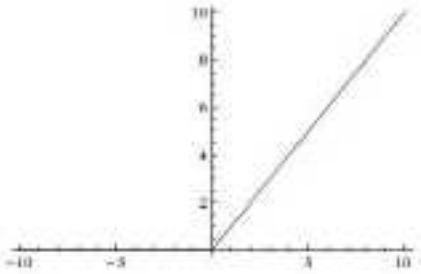
Pooling Layer

Pooling layer: to reduce the size of the input
Usually using the max value in the block(2*2 most usually) to replace the block itself





ReLu Layer



- ReLu function:

  A(x) = max(0, x)
- A nonlinear function

  Any function can be approximated with combinations of ReLu
- Not bounded

  Can blow up activation
- Sparsity of activation

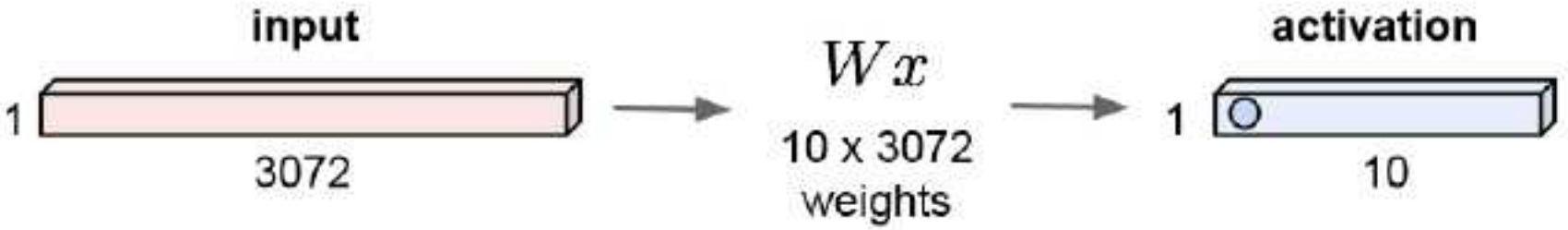
  50% neurons are not activated for randomly initialized models
- Less computational expensive

  Useful for deep networks
- Dying ReLu problem

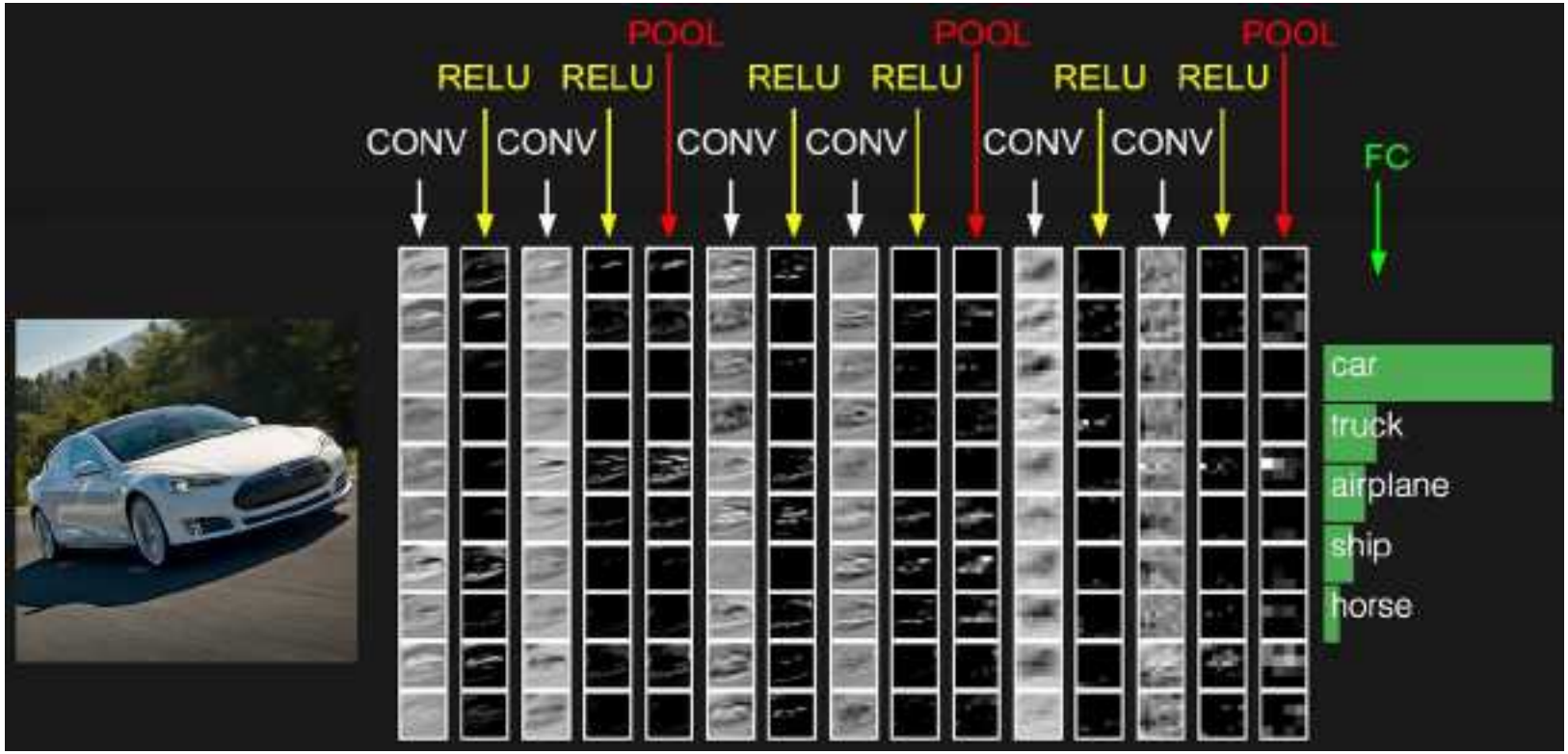
  No vanishing gradients, but dead neurons

Fully Connected Layer

32x32x3 image -> stretch to 3072 x 1



CNN Architectures



CNN

Useful websites

CS231n: Convolutional Neural Networks for Visual Recognition:
http://cs231n.github.io/

Neural Networks and Deep Learning
http://neuralnetworksanddeeplearning.com/

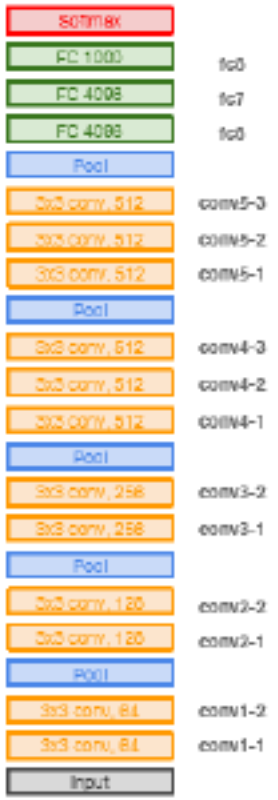
CVPR 2017 Paper interpretation
http://cvmart.net/community/article/detail/69

VGG

(not counting biases)

INPUT: [224x224x3] memory: 224*224*3=150K params: 0
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*3)*64 = 1,728
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*64)*64 = 36,864
POOL2: [112x112x64] memory: 112*112*64=800K params: 0
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*64)*128 = 73,728
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*128)*128 = 147,456
POOL2: [56x56x128] memory: 56*56*128=400K params: 0
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*128)*256 = 294,912
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
POOL2: [28x28x256] memory: 28*28*256=200K params: 0
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*256)*512 = 1,179,648
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*512)*512 = 2,359,296
POOL2: [14x14x512] memory: 14*14*512=100K params: 0
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
CONV3-512: [14x14x512] memory: 14*14*512=100K params: (3*3*512)*512 = 2,359,296
POOL2: [7x7x512] memory: 7*7*512=25K params: 0
FC: [1x1x4096] memory: 4096 params: 7*7*512*4096 = 102,760,448
FC: [1x1x4096] memory: 4096 params: 4096*4096 = 16,777,216
FC: [1x1x1000] memory: 1000 params: 4096*1000 = 4,096,000

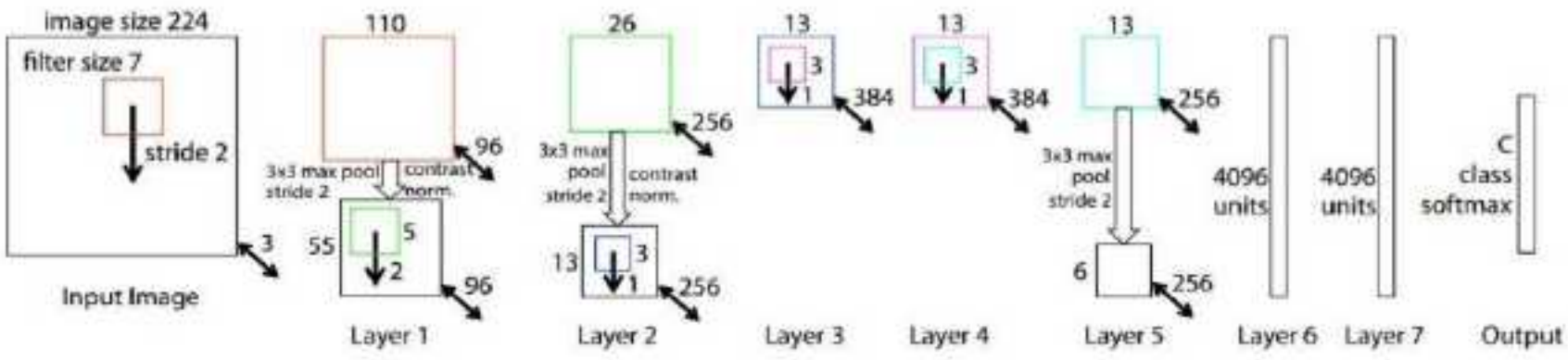
TOTAL memory: 24M * 4 bytes ~= 96MB / image (only forward! ~*2 for bwd)
TOTAL params: 138M parameters



VGG16

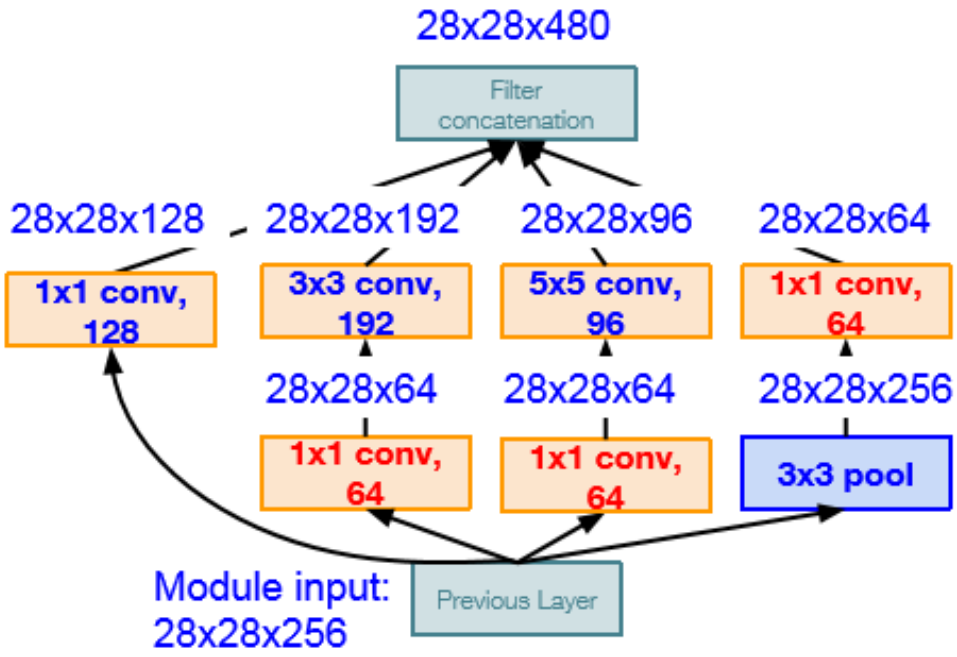
Common names

AlexNet/ZFNet



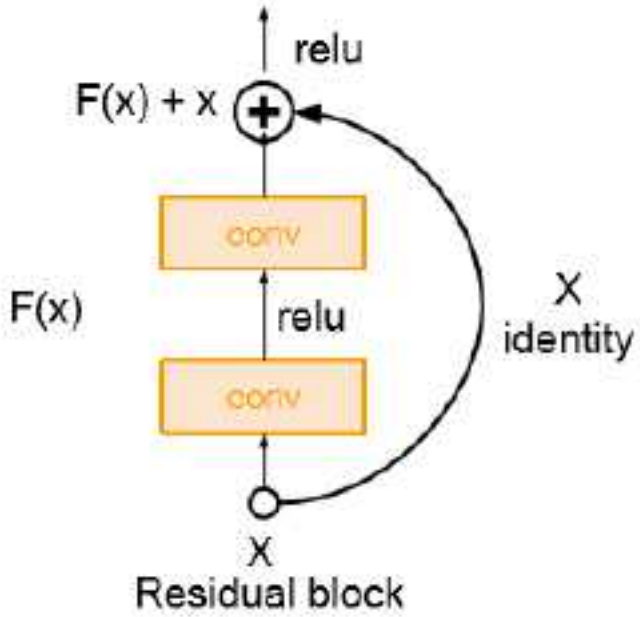
A large, deep convolutional neural network to classify the 1.3 million high-resolution images in the LSVRC-2010 ImageNet training set into the 1000 different classes http://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks

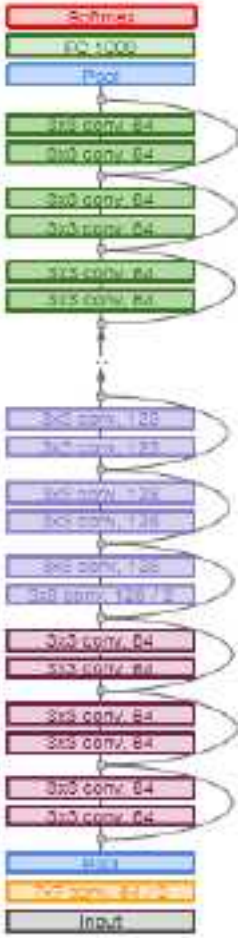
GoogleNet



Inception Module reduced a huge number of parameters in the network (4M, compared to AlexNet with 60M), using Average Pooling instead of Fully Connected layers at the top of the ConvNet, eliminating a large amount of parameters that do not seem to matter much. https://arxiv.org/pdf/1409.4842.pdf

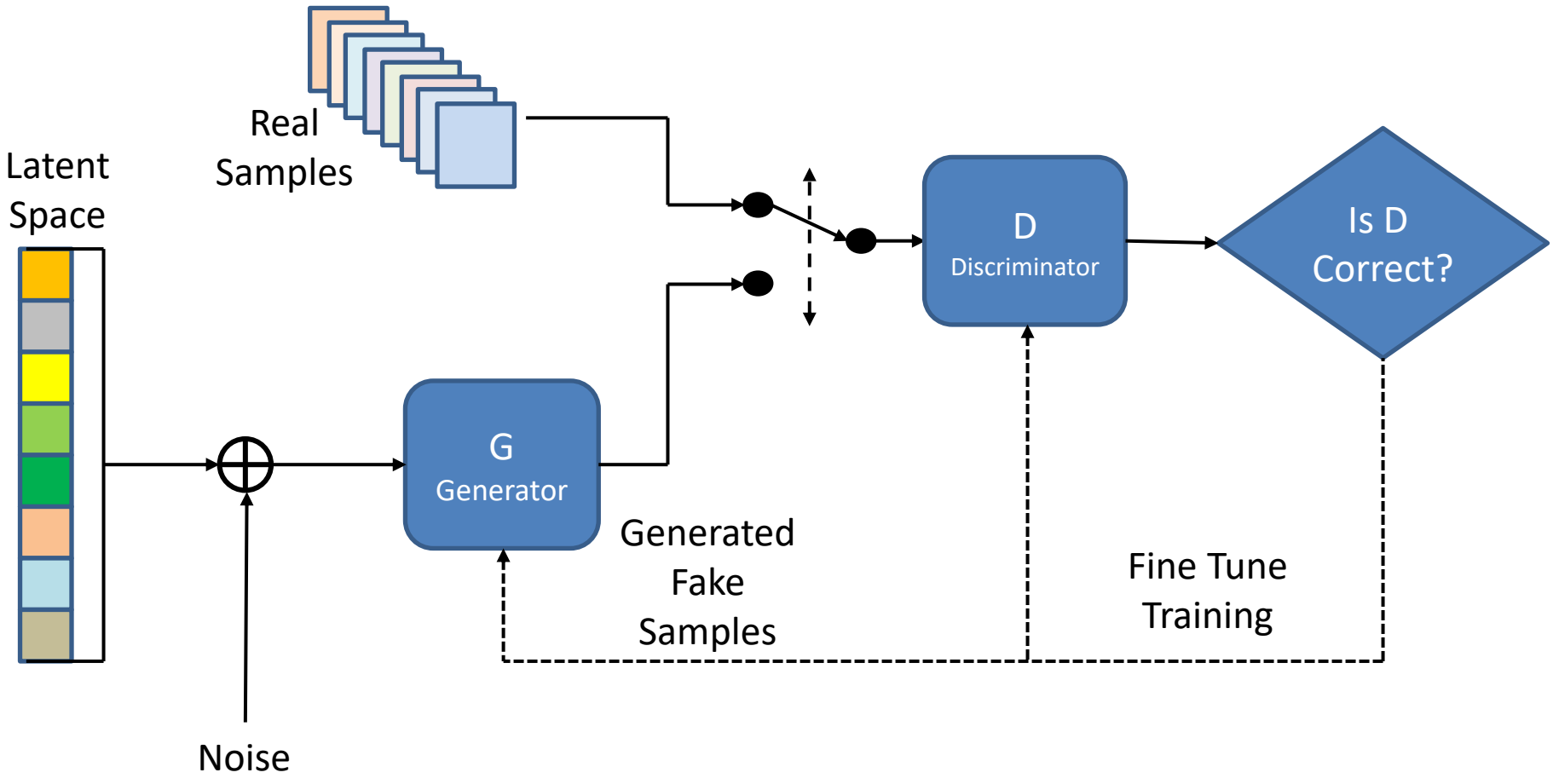
ResNet



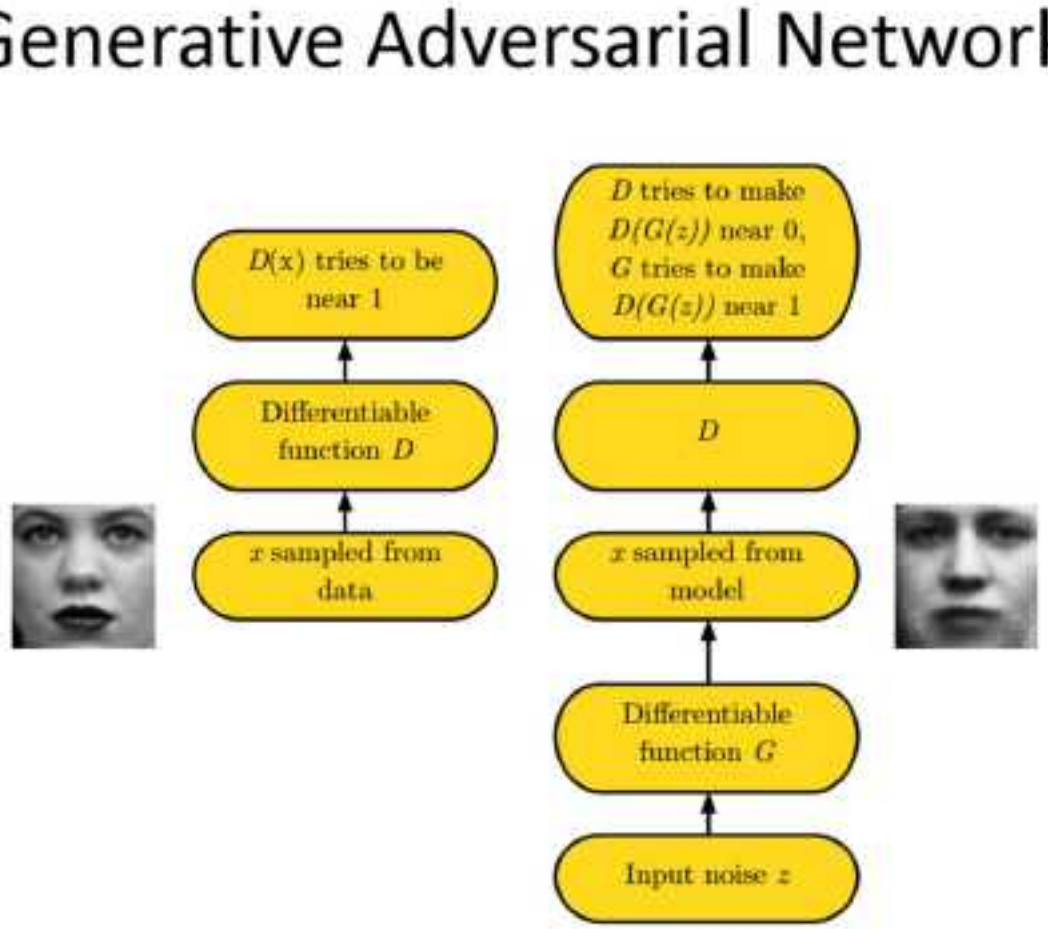


Deep Residual Learning for Image Recognition
https://arxiv.org/pdf/1512.03385.pdf

Generative Adversarial Networks



Generative Adversarial Networks



GAN

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

  for k steps **do**

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

  end for

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for

The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

Generative Adversarial Nets
https://arxiv.org/pdf/1406.2661.pdf

Summary

- Feedforward Network Functions
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