Learning and Generalization in Artificial Neural Networks

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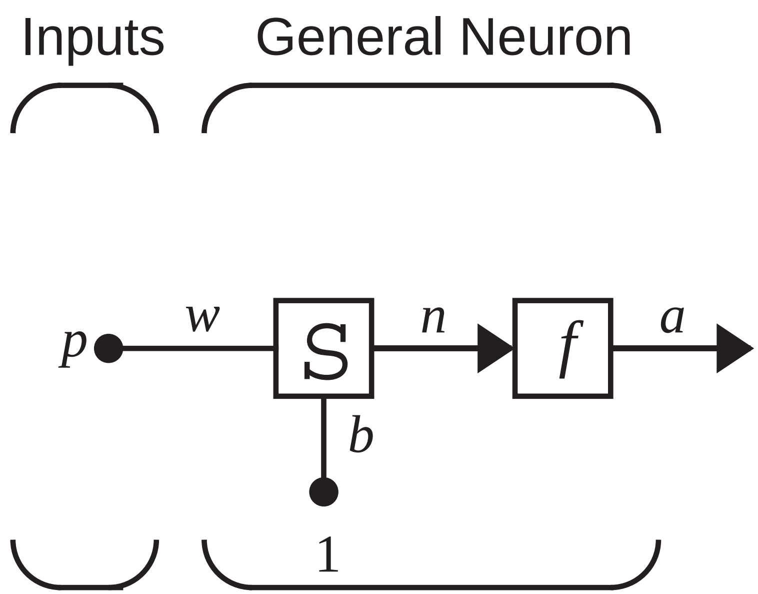
A cat that once sat on a hot stove
will never again sit on a hot stove
or on a cold one either.

Mark Twain

Outline

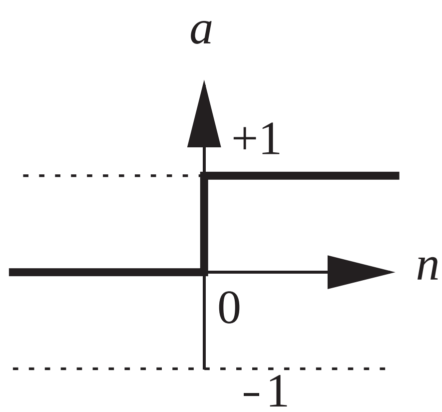
- What is an Artificial Neural Network?
- Nonlinear Regression
- Generalization
- Techniques for Improving Generalization
- Regularization
  - Bayesian Regularization
- Early Stopping
- Relationship Between Early Stopping and Regularization
- Summary

Single-Input Neuron



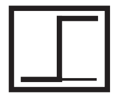
$$a = f(wp + b)$$

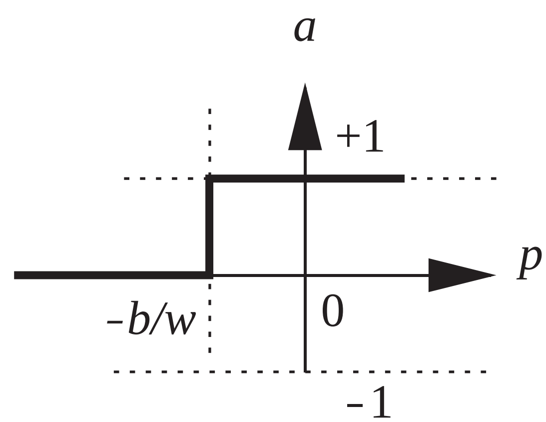
Transfer Functions



$a = hardlim(n)$

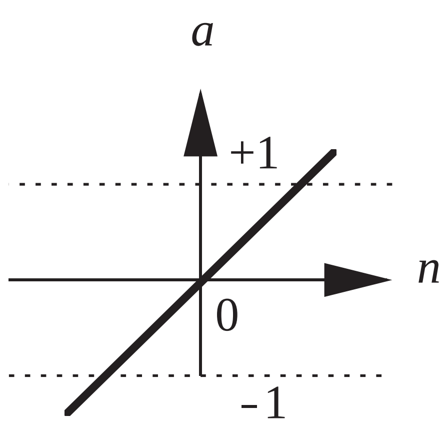
Hard Limit Transfer Function





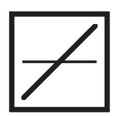
$a = hardlim(wp + b)$

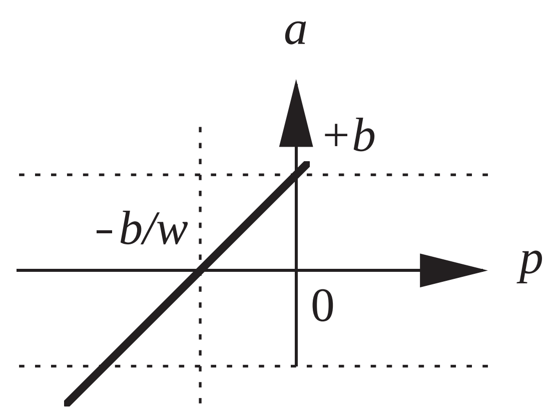
Single-Input *hardlim* Neuron



$a = purelin(n)$

Linear Transfer Function

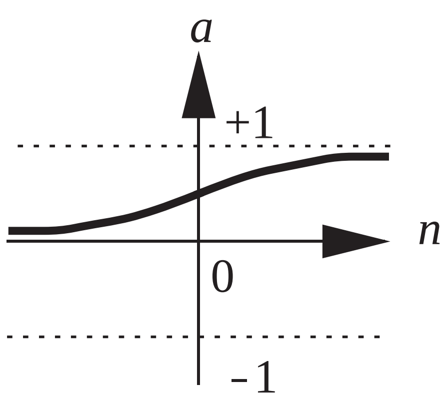


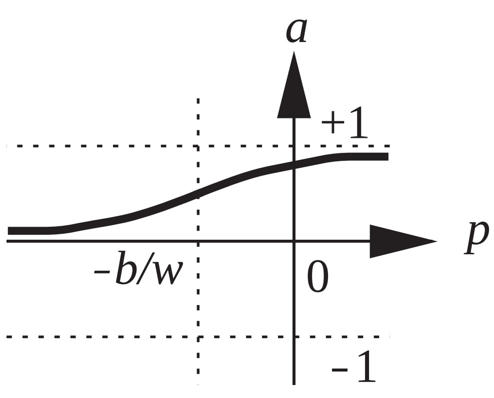


$a = purelin(wp + b)$

Single-Input *purelin* Neuron

Transfer Functions





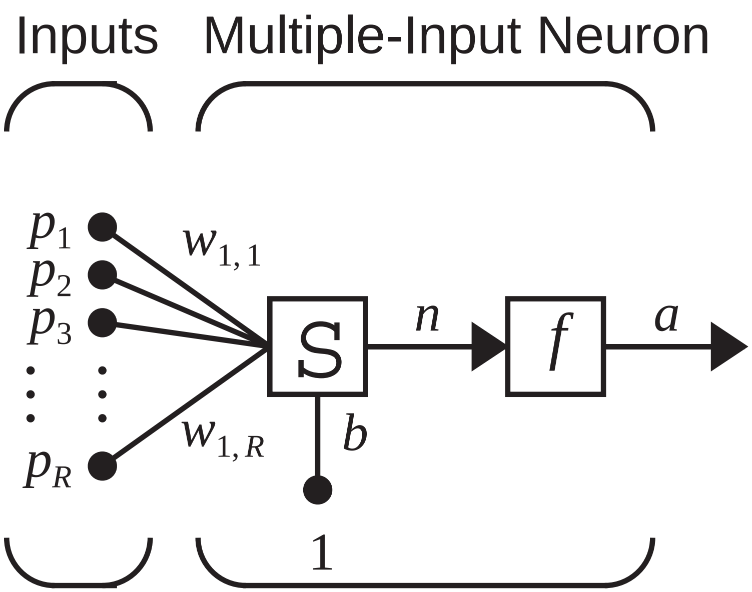
$$a = logsig(n)$$

Log-Sigmoid Transfer Function

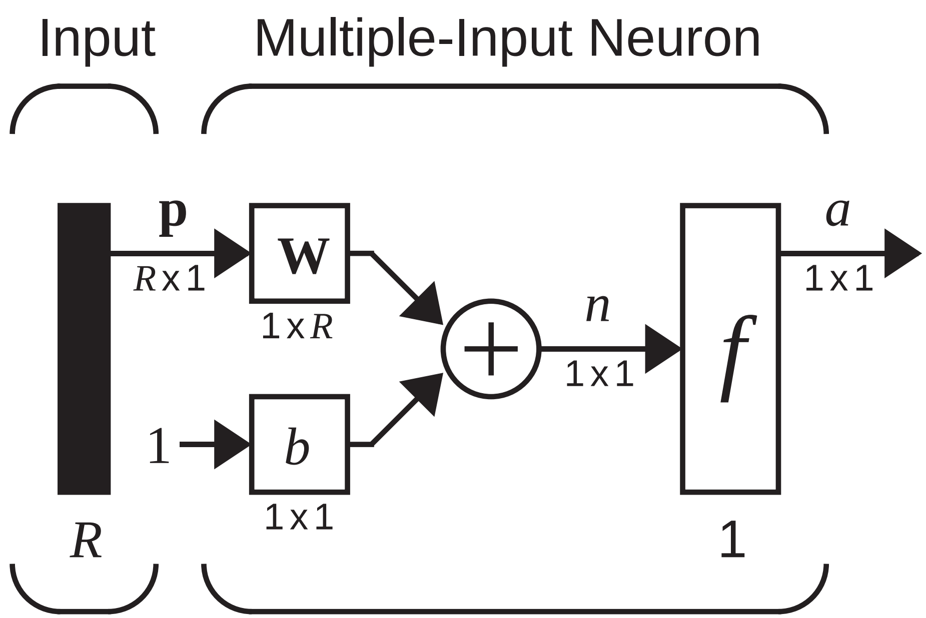
$$a = logsig(wp + b)$$

Single-Input *logsig* Neuron

Multiple-Input Neuron



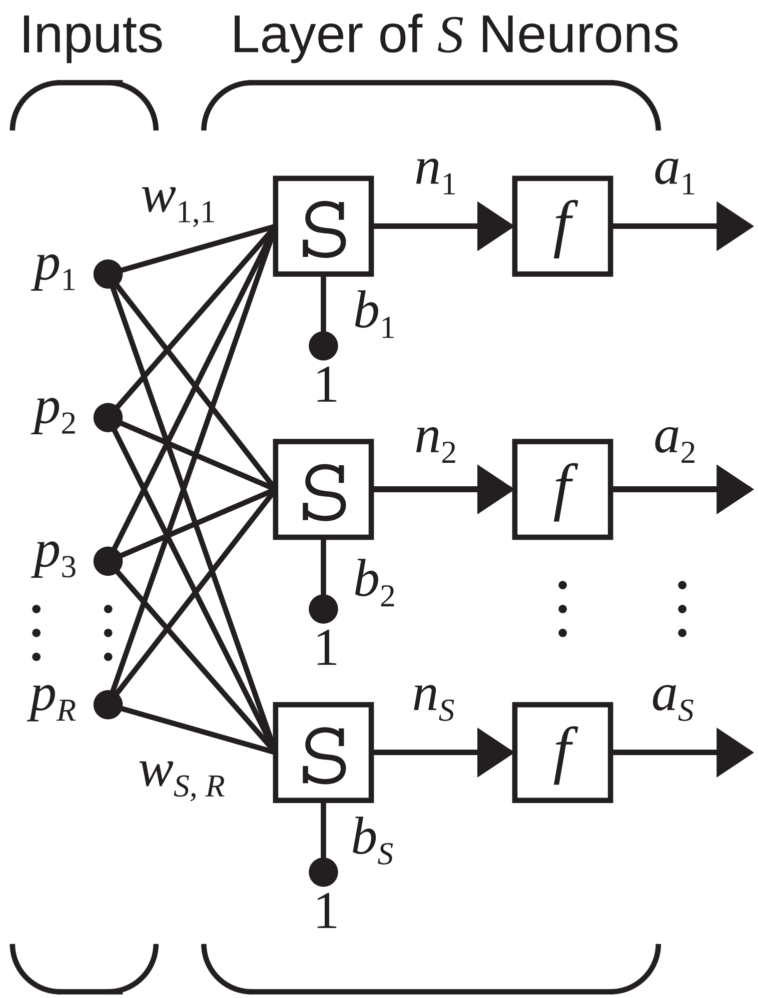
$a = f(\mathbf{W}\mathbf{p} + b)$



$a = f(\mathbf{W}\mathbf{p} + b)$

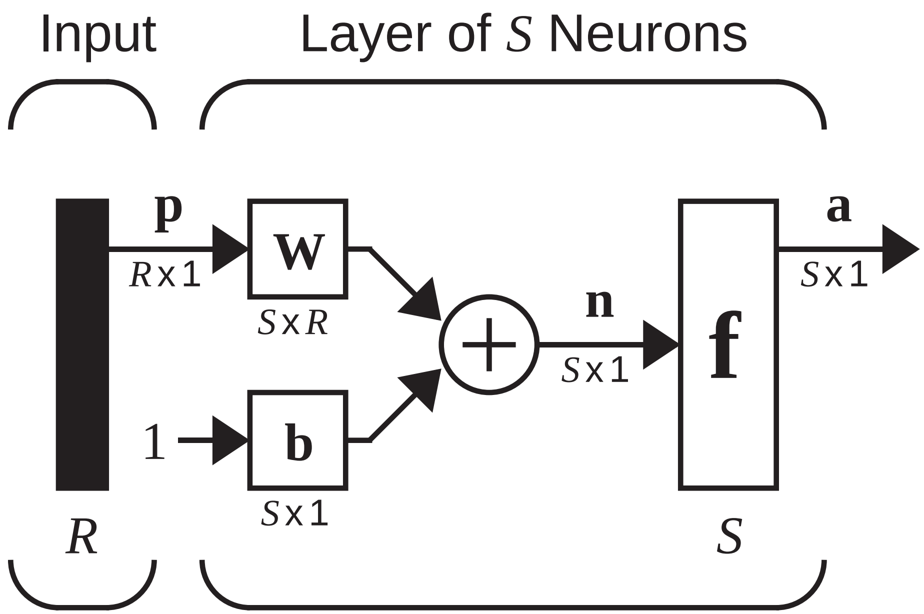
Abbreviated Notation

Layer of Neurons



$$\mathbf{a} = \mathbf{f}(\mathbf{Wp} + \mathbf{b})$$

Abbreviated Notation

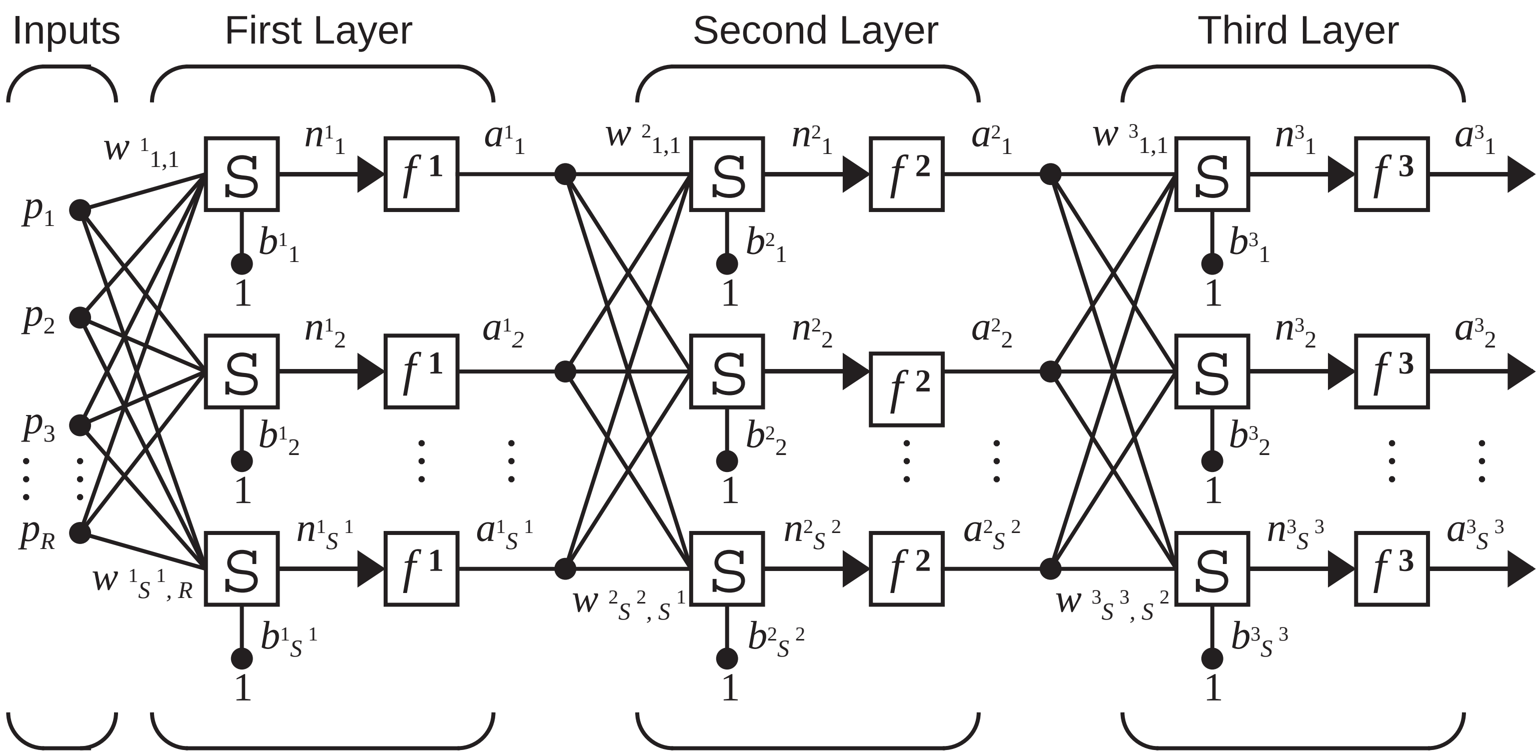


$$\mathbf{a} = \mathbf{f}(\mathbf{W}\mathbf{p} + \mathbf{b})$$

$$\mathbf{W} = \begin{bmatrix} w_{1,1} & w_{1,2} & \dots & w_{1,R} \\ w_{2,1} & w_{2,2} & \dots & w_{2,R} \\ \vdots & \vdots & & \vdots \\ w_{S,1} & w_{S,2} & \dots & w_{S,R} \end{bmatrix}$$

$$\mathbf{p} = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_R \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_S \end{bmatrix} \quad \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_S \end{bmatrix}$$

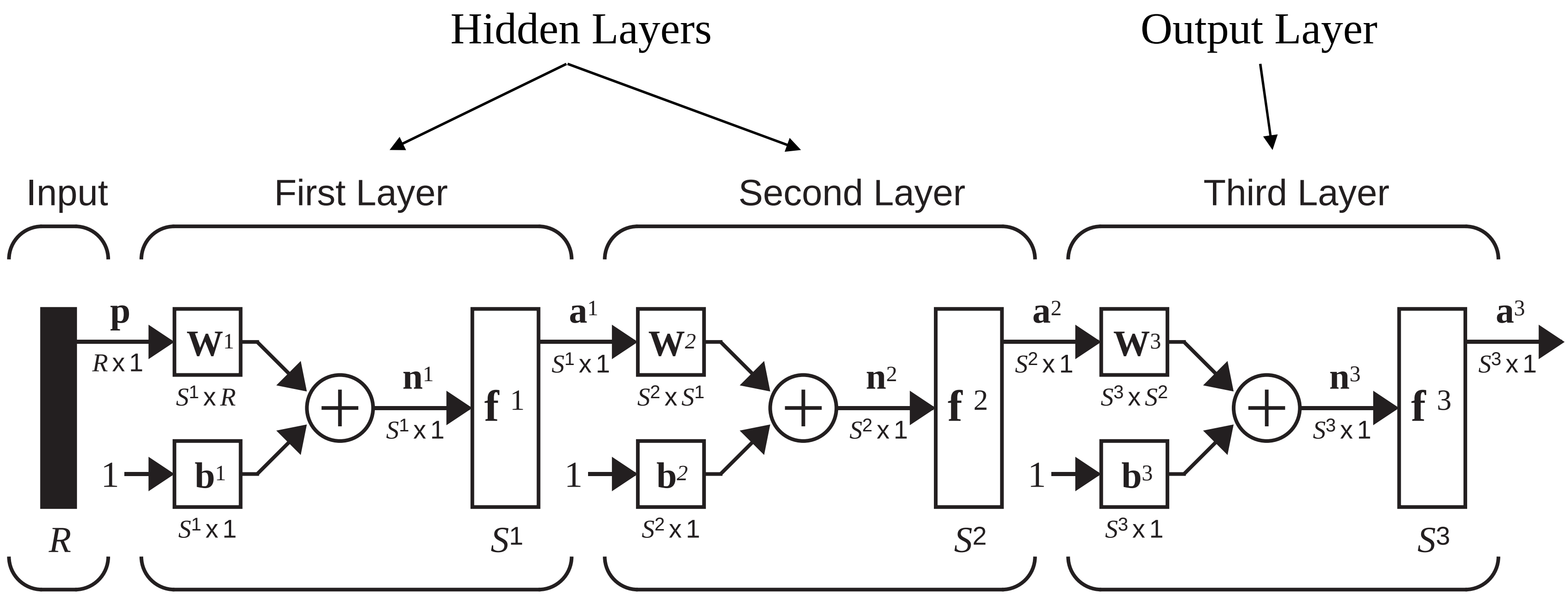
Multilayer Network



$$\mathbf{a}^1 = \mathbf{f}^1(\mathbf{W}^1\mathbf{p} + \mathbf{b}^1) \qquad \mathbf{a}^2 = \mathbf{f}^2(\mathbf{W}^2\mathbf{a}^1 + \mathbf{b}^2) \qquad \mathbf{a}^3 = \mathbf{f}^3(\mathbf{W}^3\mathbf{a}^2 + \mathbf{b}^3)$$

$$\mathbf{a}^3 = \mathbf{f}^3(\mathbf{W}^3\mathbf{f}^2(\mathbf{W}^2\mathbf{f}^1(\mathbf{W}^1\mathbf{p} + \mathbf{b}^1) + \mathbf{b}^2) + \mathbf{b}^3)$$

Abbreviated Notation



$\mathbf{a}^1 = \mathbf{f}^1(\mathbf{W}^1\mathbf{p} + \mathbf{b}^1)$ $\mathbf{a}^2 = \mathbf{f}^2(\mathbf{W}^2\mathbf{a}^1 + \mathbf{b}^2)$ $\mathbf{a}^3 = \mathbf{f}^3(\mathbf{W}^3\mathbf{a}^2 + \mathbf{b}^3)$

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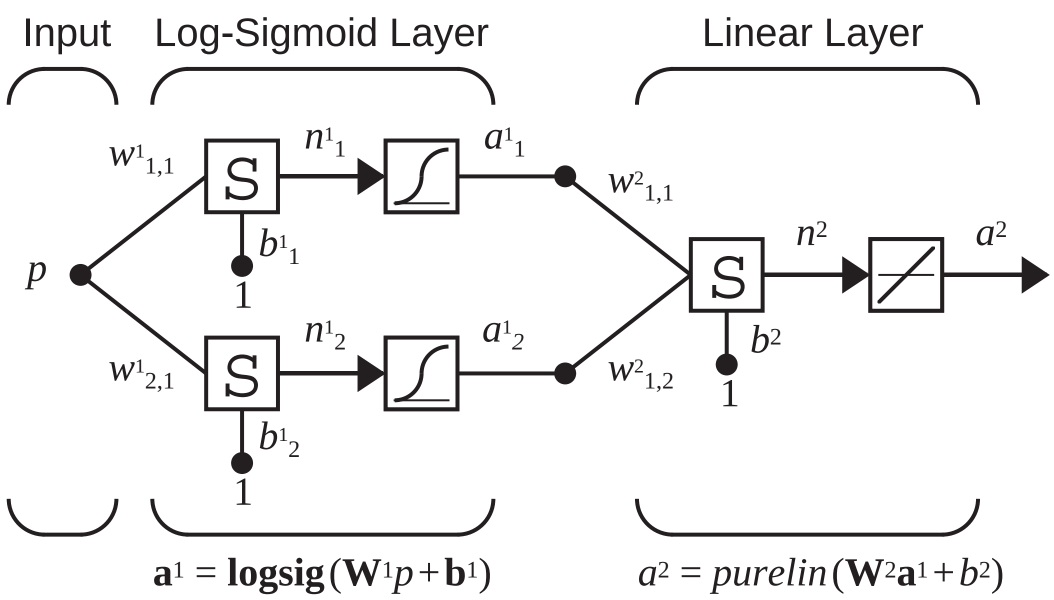
Function Approximation Example



$$f^1(n) = \frac{1}{1 + e^{-n}}$$

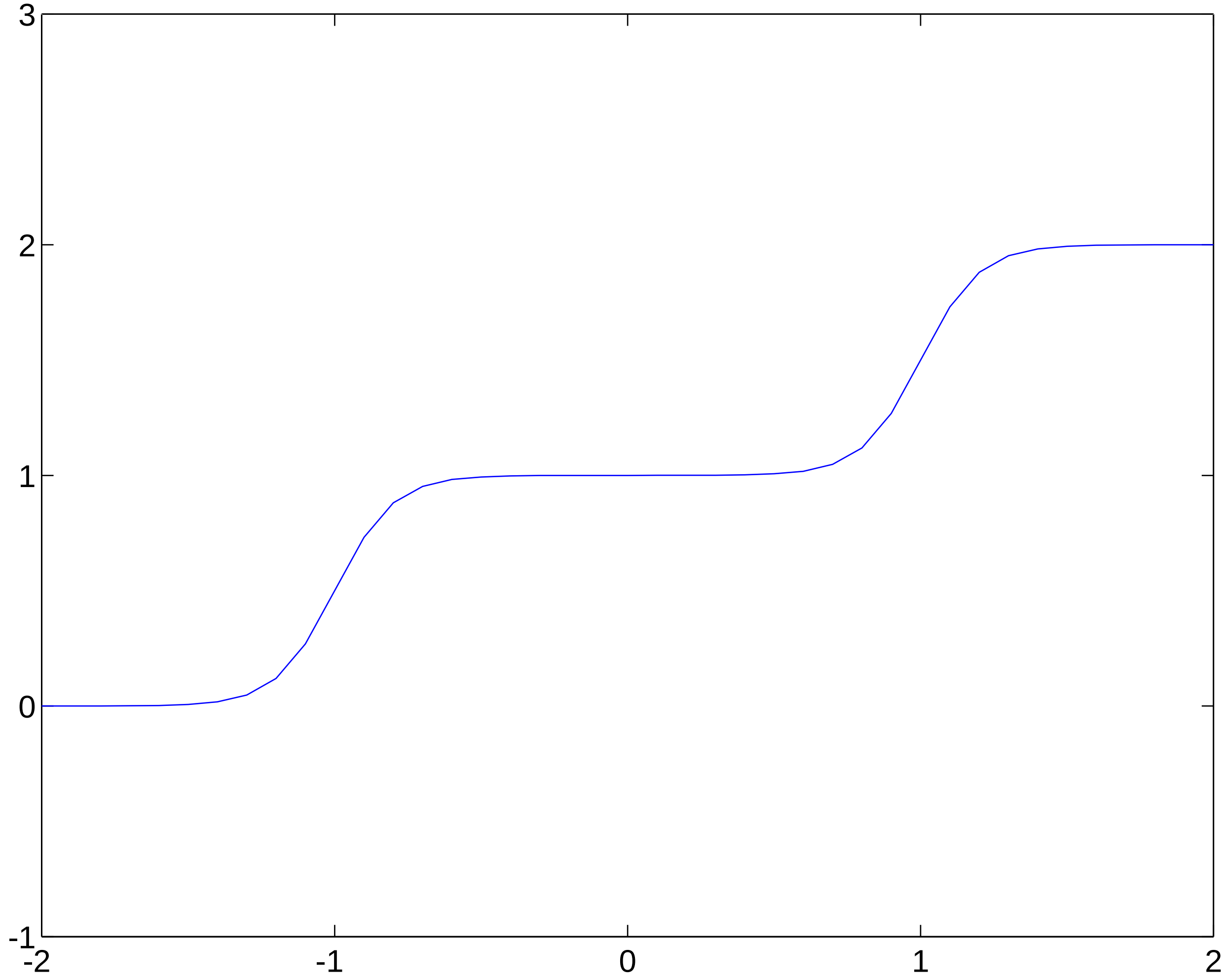
$$f^2(n) = n$$

Nominal Parameter Values

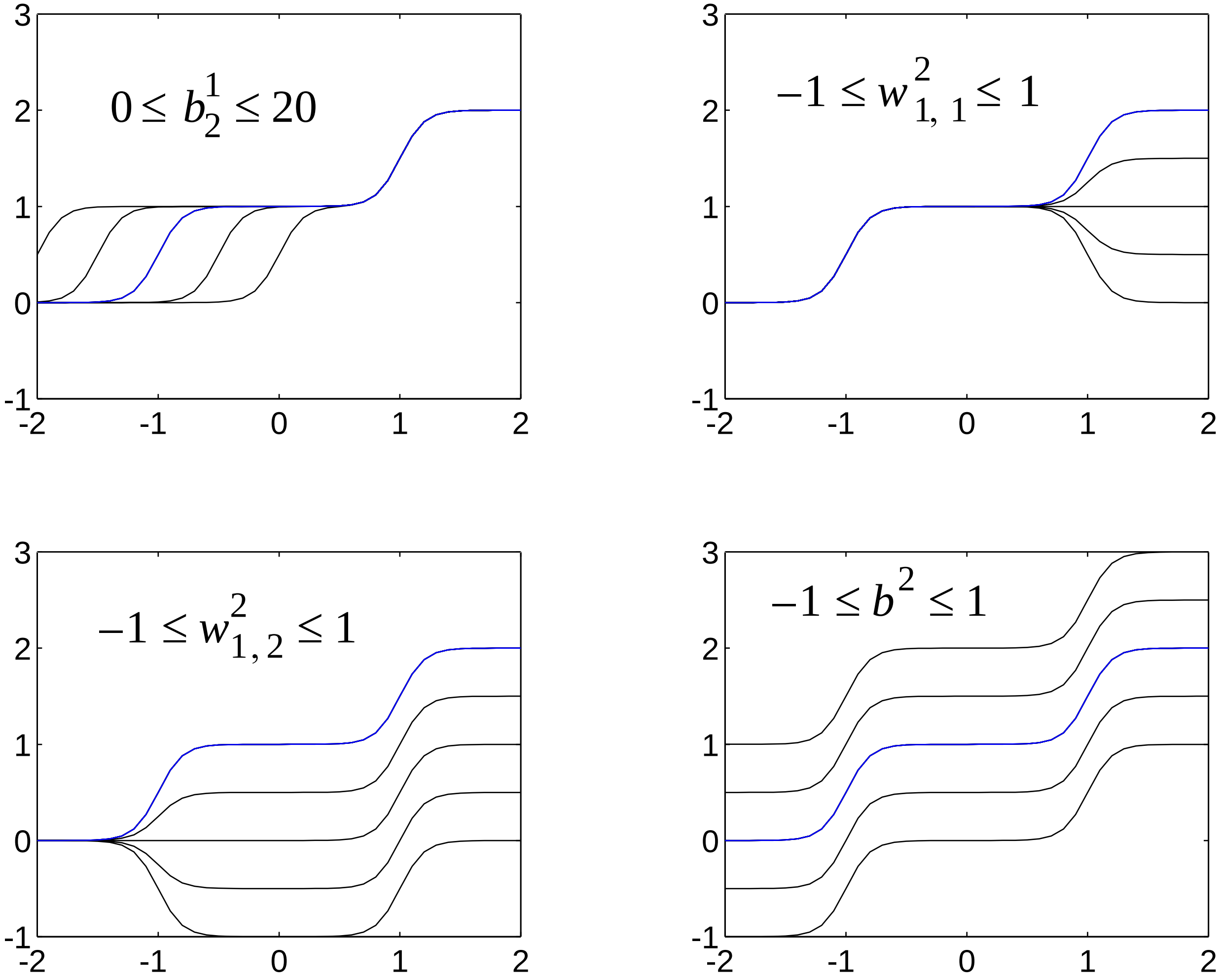
$$w^1_{1,1} = 10 \qquad w^1_{2,1} = 10 \qquad b^1_1 = -10 \qquad b^1_2 = 10$$

$$w^2_{1,1} = 1 \qquad w^2_{1,2} = 1 \qquad b^2 = 0$$

Nominal Response



Parameter Variations

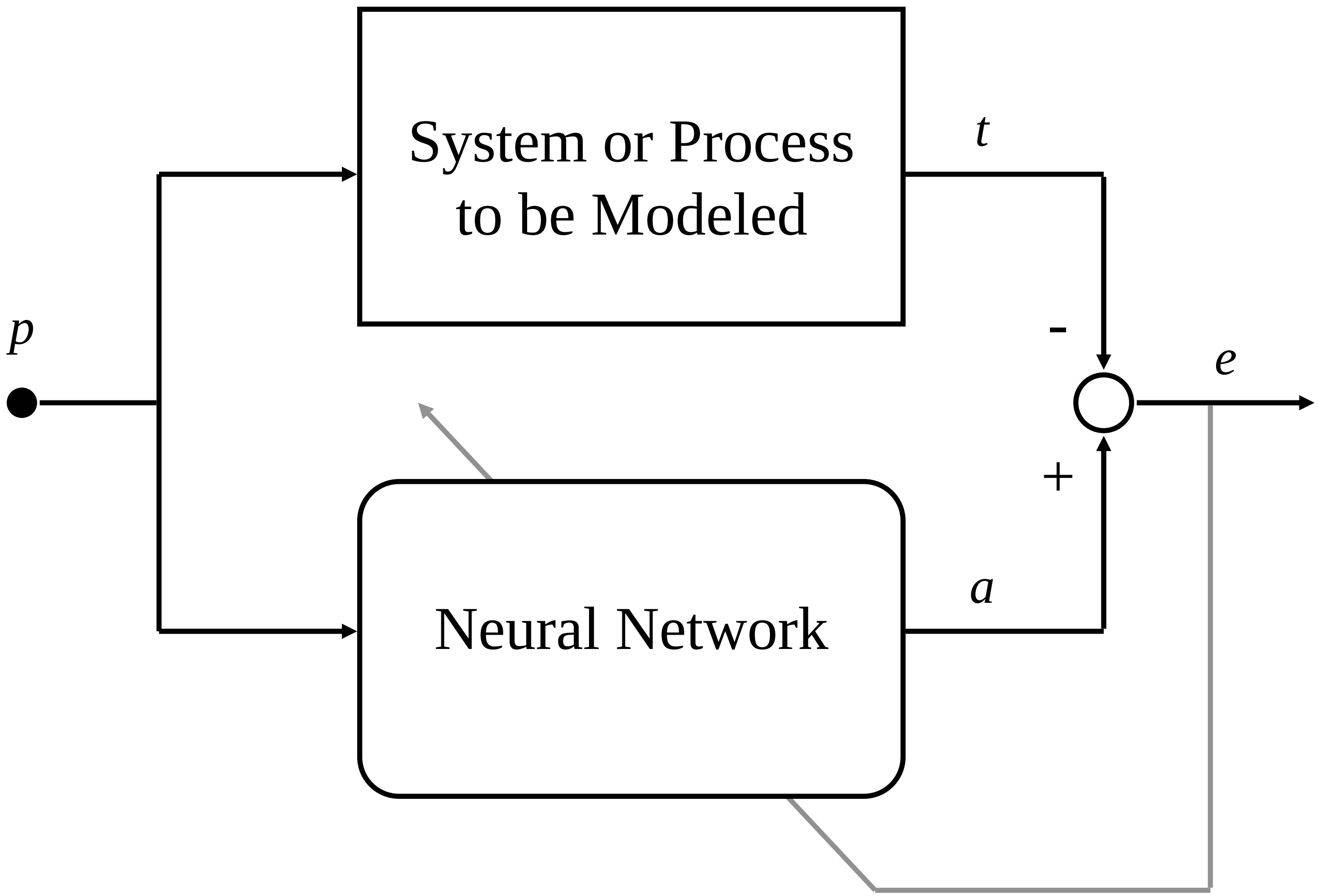


Universal Approximator

A two-layer network with a bounded, monotone-increasing transfer function in the first layer and a linear transfer function in the second layer can approximate any continuous function to an arbitrary accuracy over a bounded interval, given a sufficient number of neurons in the first layer.

Cybenko (1988)
Weierstrass (1885)

Neural Network Training



Problem Statement

Training Set

$$\{p_1, t_1\}, \{p_2, t_2\}, \dots, \{p_n, t_n\}$$

Target Generation

$$t_i = g(p_i) + \varepsilon_i$$

Performance Index for Training

$$F = E_D = \sum_{i=1}^{n} (t_i - a_i)^2$$

Regression Output

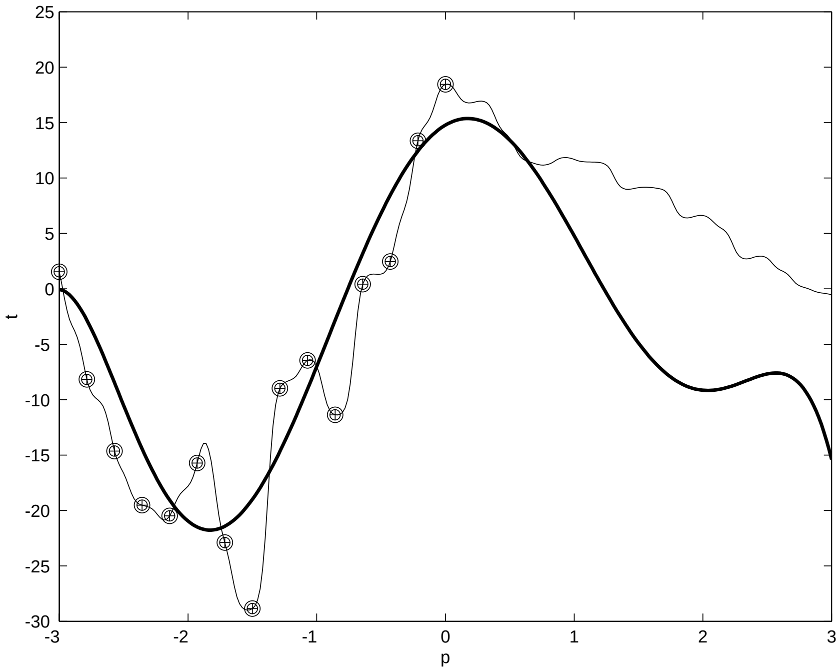
Gradient Descent Optimization

$$w_{i,j}^m(k+1) = w_{i,j}^m(k) - \alpha \frac{\partial F}{\partial w_{i,j}^m} \qquad b_i^m(k+1) = b_i^m(k) - \alpha \frac{\partial F}{\partial b_i^m}$$

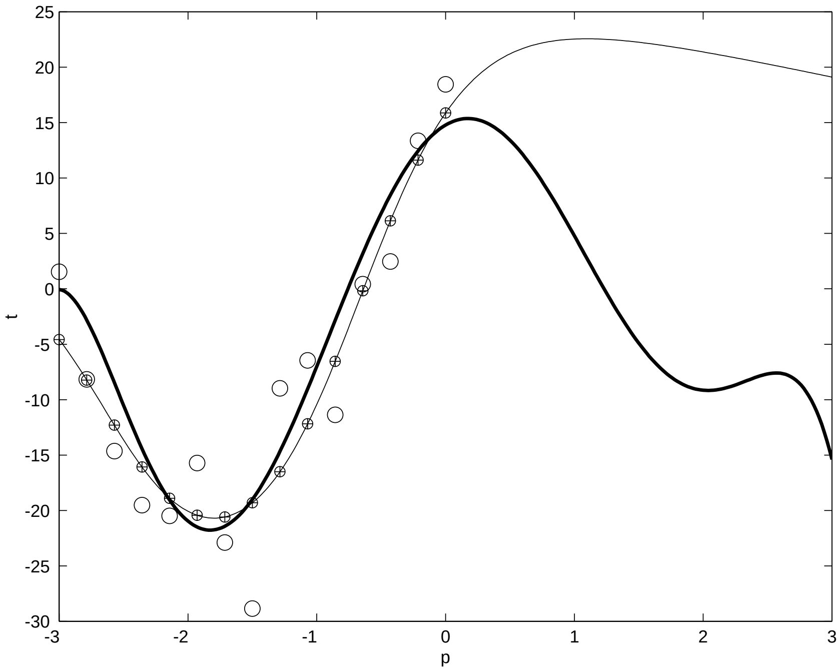
Modeling Problems

- Overfitting
- Extrapolation

Overfitting & Extrapolation



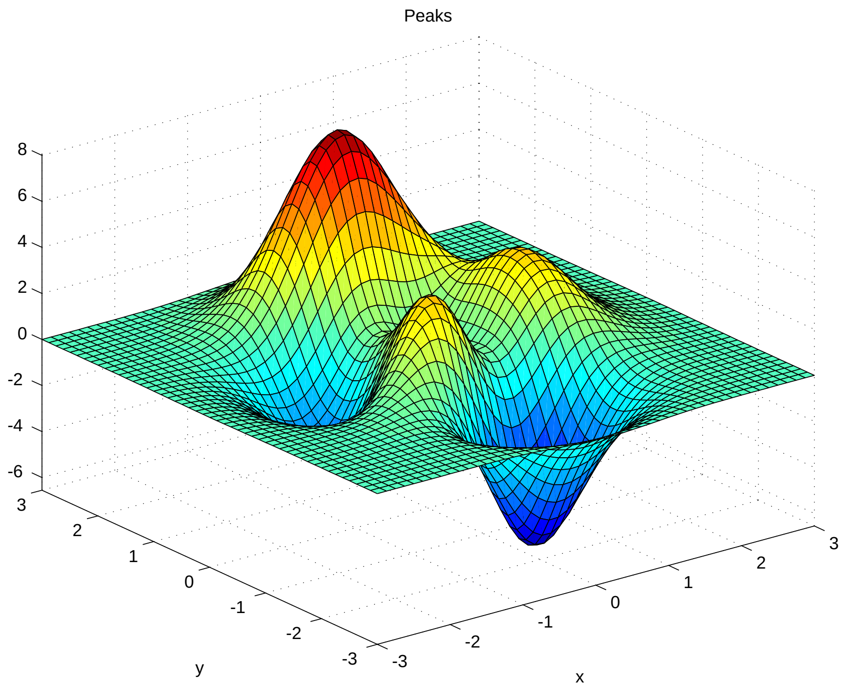
Extrapolation



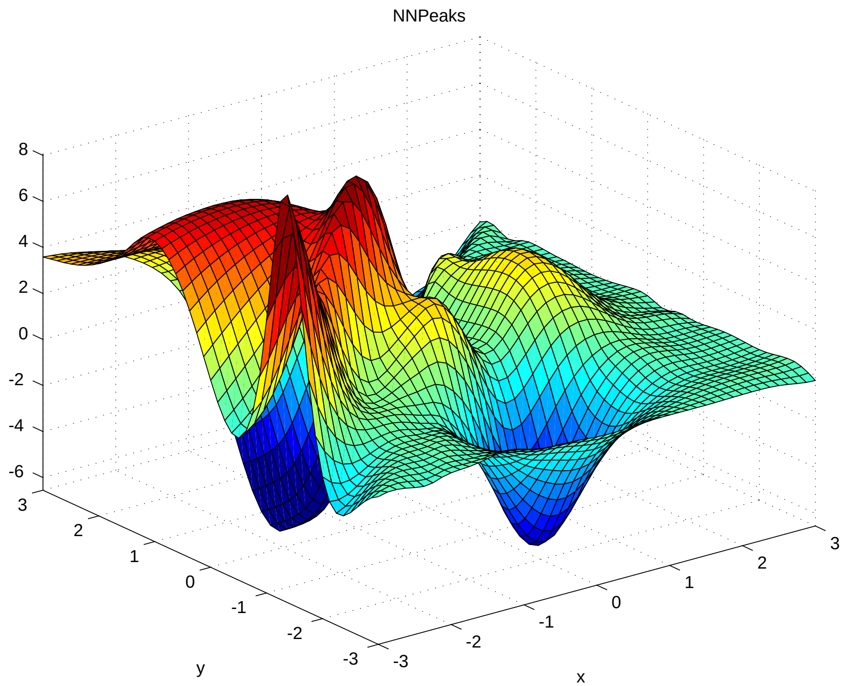
Two-Input Example

Extrapolation

True Function



Network Model



Generalization

- The network input-output mapping is accurate for the training data and for test data never seen before.
- The network interpolates well.

Cause of Overfitting

Poor generalization is caused by using a network that is too complex (too many neurons/parameters). To have the best performance we need to find the least complex network that can represent the data (Occam's Razor).

Methods for Improving Generalization

- Pruning (removing neurons) until the performance is degraded.
- Growing (adding neurons) until the performance is adequate.
- Regularization
- Validation Methods

Regularization

Standard Performance Measure

$$F = E_D$$

Performance Measure with Regularization

$$F = \beta E_D + \alpha E_W$$

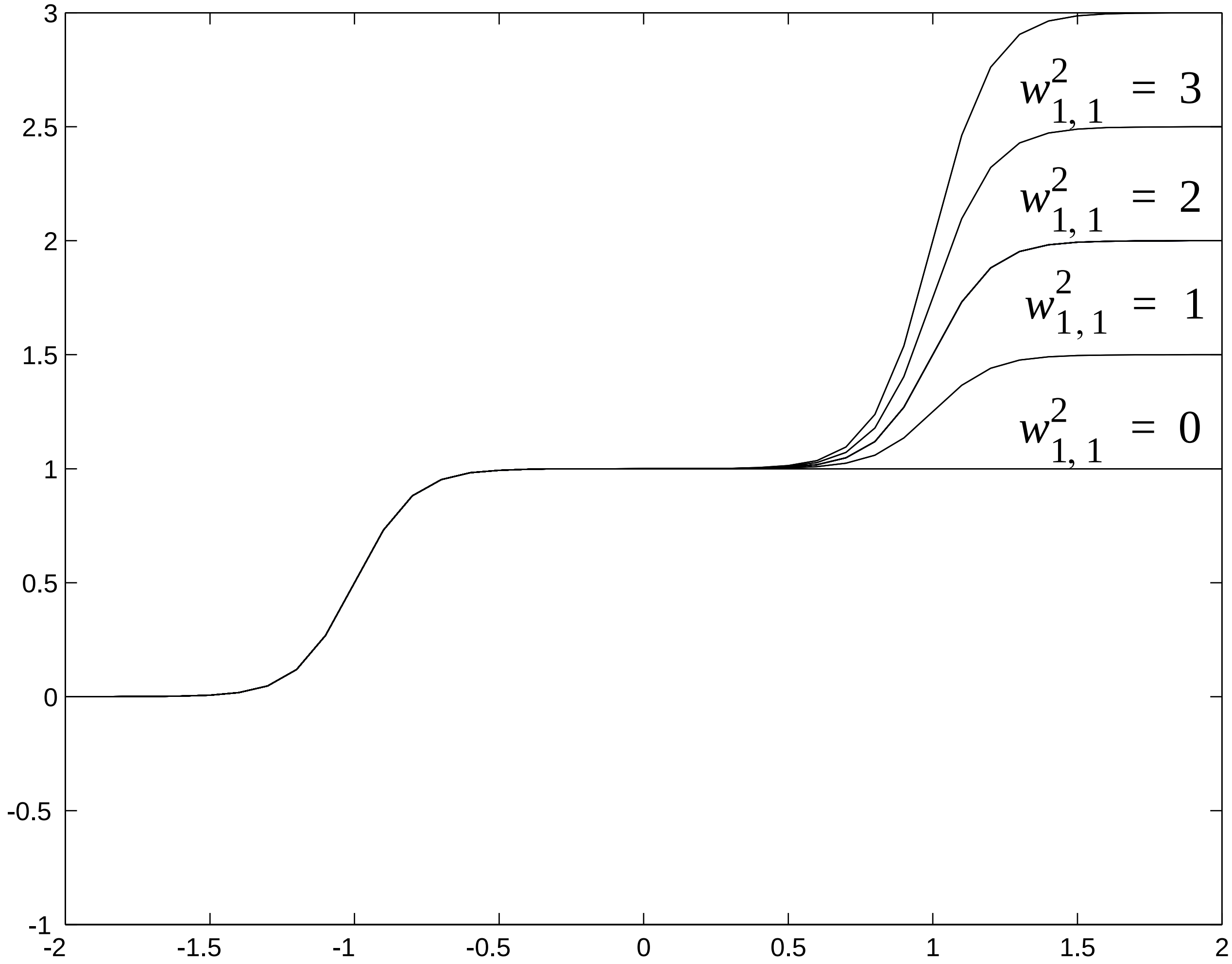
Complexity Penalty

where

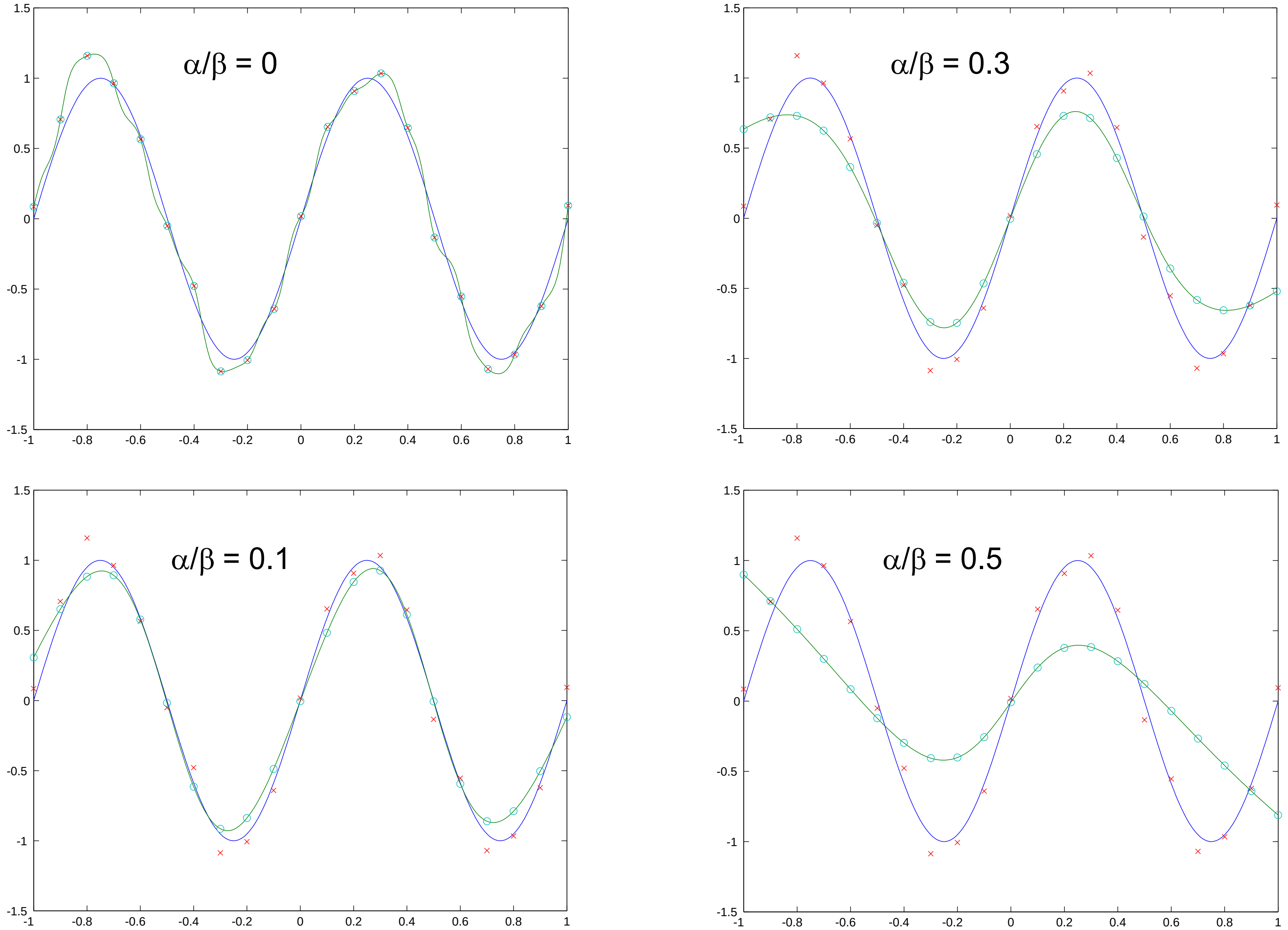
$$E_W = \sum_{i=1}^{N} w_i^2$$

(Smaller weights means a smoother function.)

Effect of Weight Changes



Effect of Regularization



NN Bayesian Framework

(MacKay 92)

$$\underbrace{P(\mathbf{w} \mid D, \alpha, \beta, M)}_{\text{Posterior (MP)}} = \frac{\underbrace{P(D \mid \mathbf{w}, \beta, M)}_{\text{Likelihood (ML)}}\,\underbrace{P(\mathbf{w} \mid \alpha, M)}_{\text{Prior}}}{\underbrace{P(D \mid \alpha, \beta, M)}_{\text{Normalization (Evidence)}}}$$

D - Data Set

M - Neural Network Model

$\mathbf{w}$ - Vector of Network Weights

Gaussian Assumptions

Gaussian Noise

$$P(D|\mathbf{w}, \beta, M) = \frac{1}{Z_D(\beta)} \exp(-\beta E_D) \qquad Z_D(\beta) = (\pi / \beta)^{n/2}$$

Gaussian Prior:

$$P(\mathbf{w}|\alpha, M) = \frac{1}{Z_W(\alpha)} \exp(-\alpha E_W) \qquad Z_W(\alpha) = (\pi / \alpha)^{N/2}$$

$$P(\mathbf{w}|D, \alpha, \beta, M) = \frac{\frac{1}{Z_W(\alpha)} \frac{1}{Z_D(\beta)} \exp(-(\beta E_D + \alpha E_W))}{\text{Normalization Factor}}$$

$$= \frac{1}{Z_F(\alpha, \beta)} \exp(-F(\mathbf{w}))$$

Minimize F to Maximize P.

Optimizing Regularization Parameters

Evidence from First Level

Second Level of Inference

$$P(\alpha, \beta | D, M) = \frac{P(D | \alpha, \beta, M) P(\alpha, \beta | M)}{P(D | M)}$$

Evidence:

$$P(D | \alpha, \beta, M) = \frac{P(D | \mathbf{w}, \beta, M) P(\mathbf{w} | \alpha, M)}{P(\mathbf{w} | D, \alpha, \beta, M)}$$

$$= \frac{\left[\frac{1}{Z_D(\beta)} \exp(-\beta E_D)\right]\left[\frac{1}{Z_W(\alpha)} \exp(-\alpha E_W)\right]}{\frac{1}{Z_F(\alpha, \beta)} \exp(-F(\mathbf{w}))}$$

$$= \frac{Z_F(\alpha, \beta)}{Z_D(\beta) Z_W(\alpha)} \cdot \frac{\exp(-\beta E_D - \alpha E_W)}{\exp(-F(\mathbf{w}))} = \frac{Z_F(\alpha, \beta)}{Z_D(\beta) Z_W(\alpha)}$$

Quadratic Approximation

The only unknown term in the evidence is Z_F. It can be approximated using a second order Taylor series expansion.

$$Z_F \approx (2\pi)^{N/2} \left(\det\left((\mathbf{H}^{\mathrm{MP}})^{-1}\right)\right)^{1/2} \exp\left(-F(\mathbf{w}^{\mathrm{MP}})\right)$$

Hessian Matrix

$$\mathbf{H} = \beta \nabla^2 E_D + \alpha \nabla^2 E_W$$

Optimum Parameters

If we make this substitution for Z_F in the expression for the evidence and then take the derivative with respect to α and β to locate the minimum we find:

$$\alpha^{\mathrm{MP}} = \frac{\gamma}{2E_W(\mathbf{w}^{\mathrm{MP}})} \qquad \beta^{\mathrm{MP}} = \frac{n-\gamma}{2E_D(\mathbf{w}^{\mathrm{MP}})}$$

Effective Number of Parameters

$$\gamma = N - 2\alpha^{\mathrm{MP}}\mathrm{tr}(\mathbf{H}^{\mathrm{MP}})^{-1}$$

Gauss-Newton Approximation

It can be expensive to compute the Hessian matrix.

Try the Gauss-Newton Approximation.

$$\mathbf{H} = \nabla^2 F(\mathbf{w}) \approx 2\beta \mathbf{J}^T \mathbf{J} + 2\alpha \mathbf{I}_N$$

This is readily available if the Levenberg-Marquardt algorithm is used for training.

Algorithm

0. Initialize α, β and the weights.

1. Take one step of Levenberg-Marquardt to minimize $F(\mathbf{w})$.

2. Compute the effective number of parameters $\gamma = N - 2\alpha \mathrm{tr}(\mathbf{H}^{-1})$, using the Gauss-Newton approximation for $\mathbf{H}$.

3. Compute new estimates of the regularization parameters $\alpha = \gamma/(2E_W)$ and $\beta = (n-\gamma)/(2E_D)$.

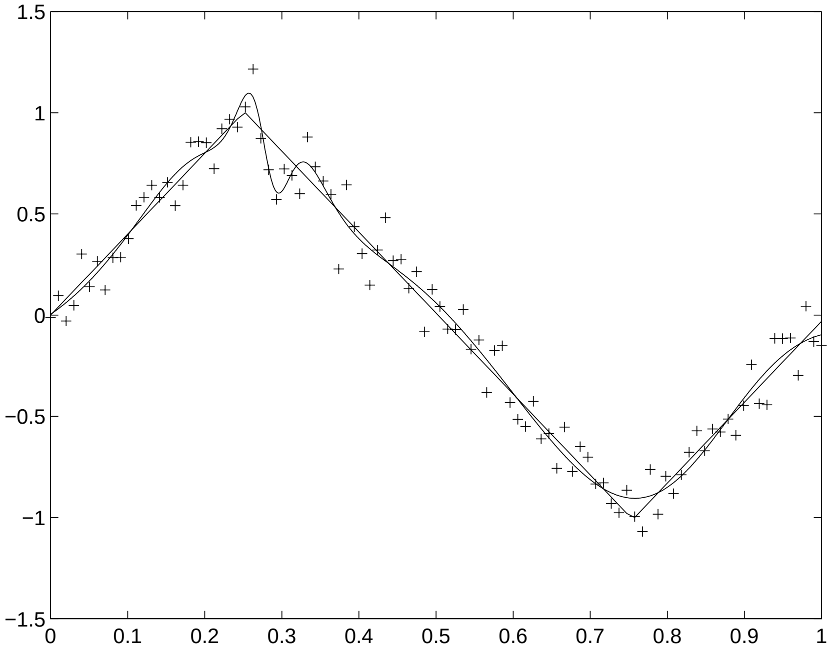
4. Iterate steps 1-3 until convergence.

Checks of Performance

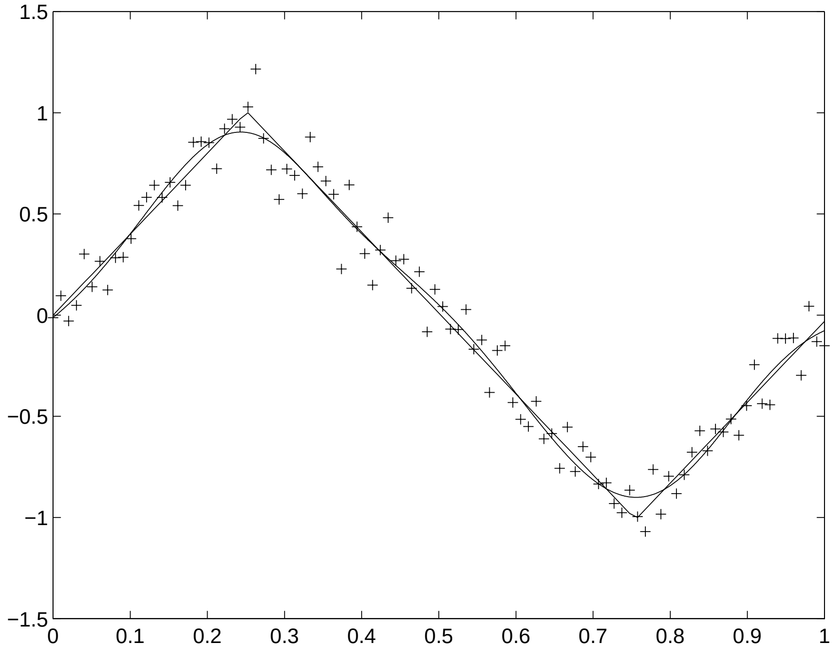
- If γ is very close to N, then the network may be too small. Add more hidden layer neurons and retrain.
- If the larger network has the same final γ, then the smaller network was large enough.
- Otherwise, increase the number of hidden neurons.
- If a network is sufficiently large, then a larger network will achieve comparable values for γ, E_D and E_W.

Simple Test Problem

1-6-1 Network
Without Regularization



1-6-1 Network
With Regularization



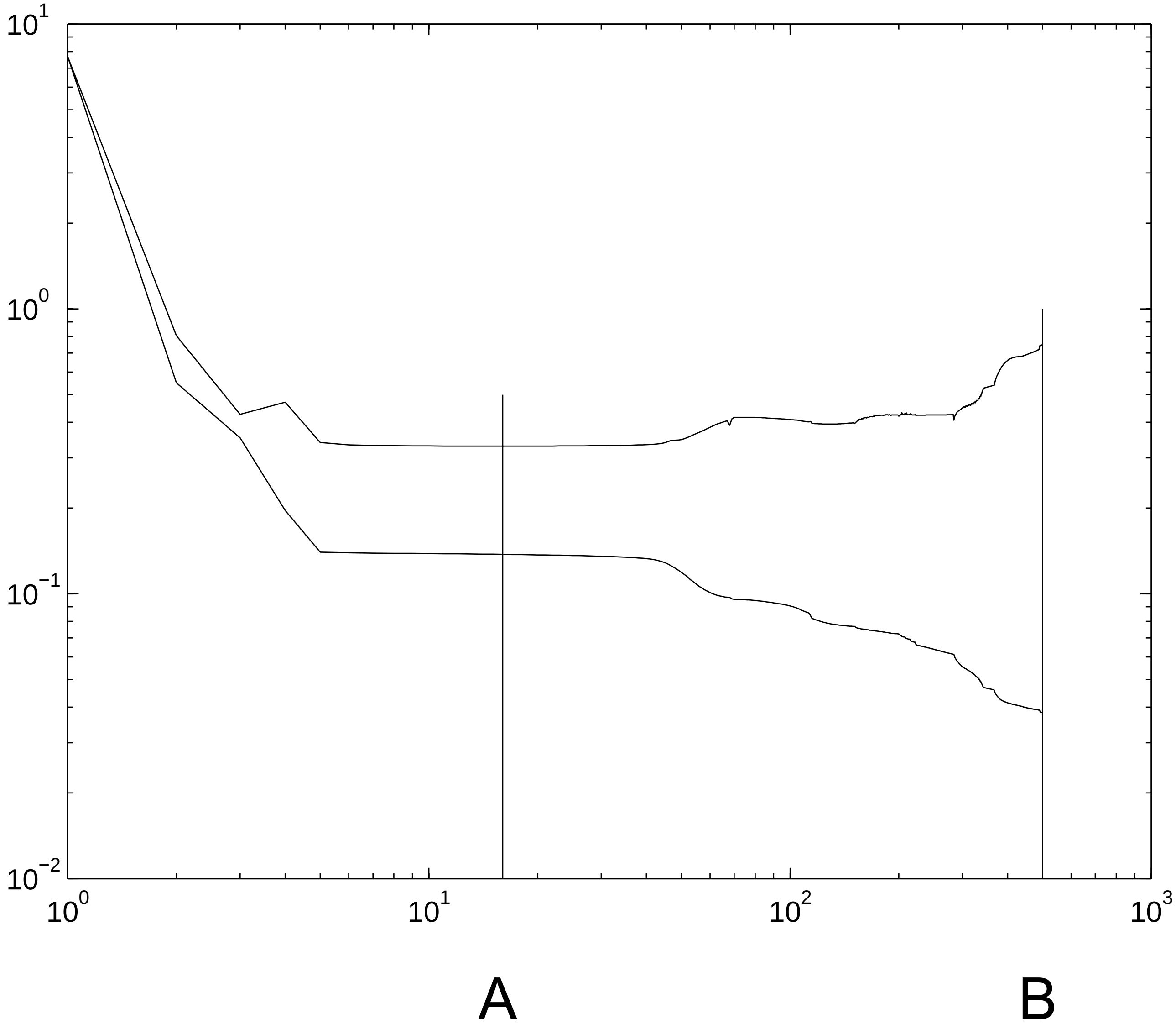
Triangle Wave Results

S	E_D	E_W	E_A	N	γ
2	1.612	203.0	0.5031	7	5.659
3	1.214	187.8	0.1954	10	8.468
4	1.144	177.0	0.1080	13	9.843
5	1.143	177.2	0.1085	16	9.906
6	1.143	177.2	0.1088	19	9.908
8	1.143	177.1	0.1091	25	9.911
10	1.142	177.1	0.1093	31	9.913
14	1.142	177.0	0.1095	43	9.915

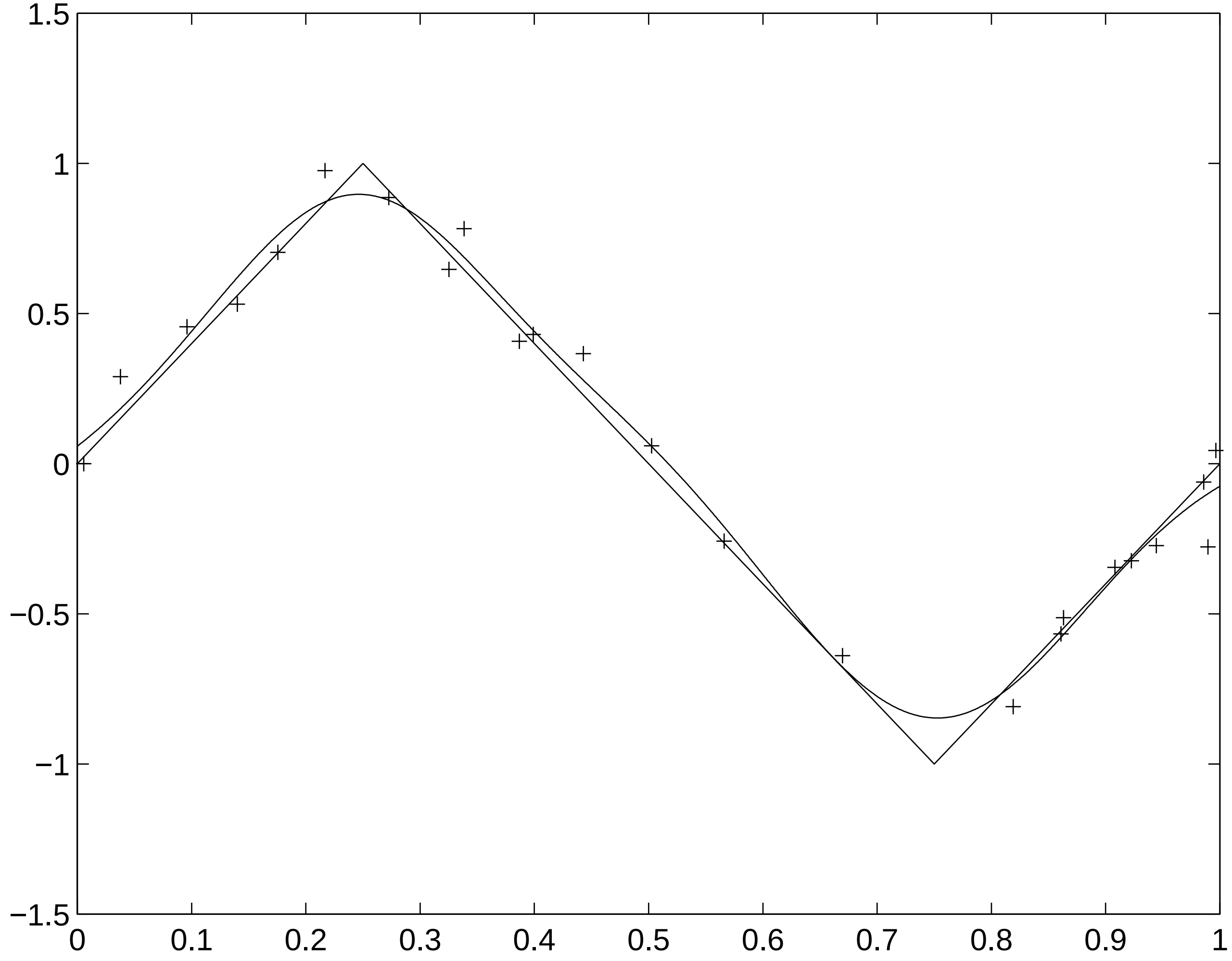
Early Stopping

- Break up data into training, *validation*, and test sets.
- Use only the training set to compute gradients and determine weight updates.
- Compute the performance on the validation set at each iteration of training.
- Stop training when the performance on the validation set goes up for a specified number of iterations.
- Use the weights which achieved the lowest error on the validation set.

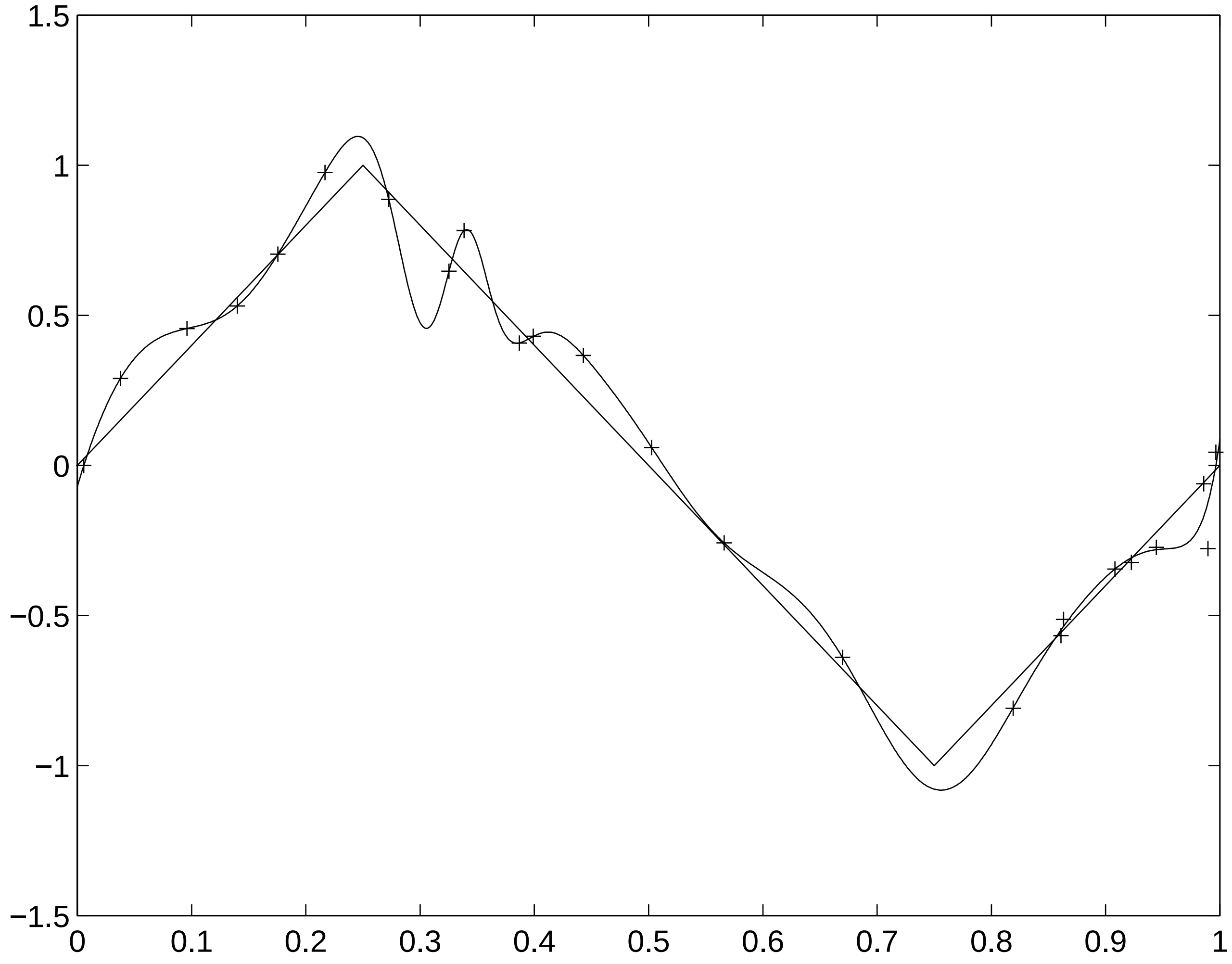
Training and Validation Error



Point A Response (Early Stopping)



Point B Response (Overfit)



Other Validation Set Uses

- Setting the regularization parameter
- Committee of networks
  - Averaging
  - Voting
- Boosting
- …

Relationship Between Early Stopping and Regularization

Quadratic Functions

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{d}^T\mathbf{x} + c \qquad \text{(Symmetric } \mathbf{A}\text{)}$$

Gradient and Hessian:

Useful properties of gradients:

$$\nabla(\mathbf{h}^T\mathbf{x}) = \nabla(\mathbf{x}^T\mathbf{h}) = \mathbf{h}$$

$$\nabla\mathbf{x}^T\mathbf{Q}\mathbf{x} = \mathbf{Q}\mathbf{x} + \mathbf{Q}^T\mathbf{x} = 2\mathbf{Q}\mathbf{x} \quad \text{(for symmetric } \mathbf{Q}\text{)}$$

Gradient of Quadratic Function:

$$\boxed{\nabla F(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{d}}$$

Hessian of Quadratic Function:

$$\boxed{\nabla^2 F(\mathbf{x}) = \mathbf{A}}$$

Eigensystem of the Hessian

Consider a quadratic function which has a stationary point at the origin, and whose value there is zero.

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}$$

Perform a similarity transform on the Hessian matrix, using the eigenvalues as the new basis vectors.

$$\mathbf{B} = \begin{bmatrix}\mathbf{z}_1 & \mathbf{z}_2 & \dots & \mathbf{z}_n\end{bmatrix}$$

Since the Hessian matrix is symmetric, its eigenvectors are orthogonal.

$$\mathbf{B}^{-1} = \mathbf{B}^T$$

$$\mathbf{A}' = [\mathbf{B}^T\mathbf{A}\mathbf{B}] = \begin{bmatrix}\lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \lambda_n\end{bmatrix} = \Lambda \qquad \mathbf{A} = \mathbf{B}\Lambda\mathbf{B}^T$$

Second Directional Derivative

$$\frac{\mathbf{p}^T \nabla^2 F(\mathbf{x}) \mathbf{p}}{\|\mathbf{p}\|^2} = \frac{\mathbf{p}^T \mathbf{A} \mathbf{p}}{\|\mathbf{p}\|^2}$$

Represent $\mathbf{p}$ with respect to the eigenvectors (new basis):

$$\mathbf{p} = \mathbf{B}\mathbf{c}$$

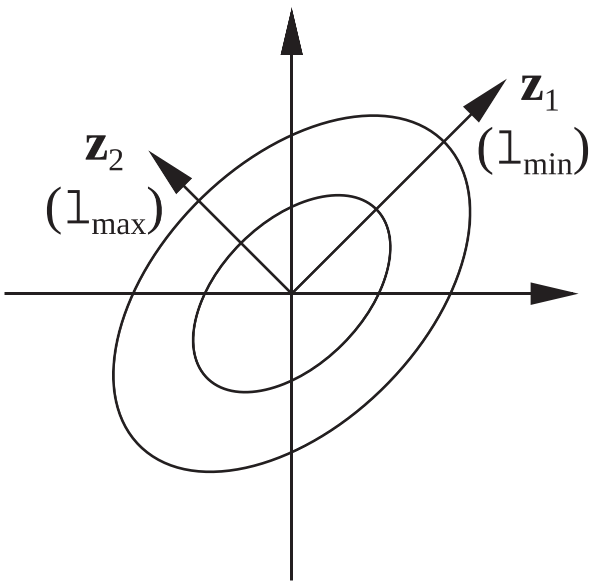
$$\frac{\mathbf{p}^T \mathbf{A} \mathbf{p}}{\|\mathbf{p}\|^2} = \frac{\mathbf{c}^T \mathbf{B}^T (\mathbf{B} \Lambda \mathbf{B}^T) \mathbf{B} \mathbf{c}}{\mathbf{c}^T \mathbf{B}^T \mathbf{B} \mathbf{c}} = \frac{\mathbf{c}^T \Lambda \mathbf{c}}{\mathbf{c}^T \mathbf{c}} = \frac{\sum_{i=1}^{n} \lambda_i c_i^2}{\sum_{i=1}^{n} c_i^2}$$

$$\lambda_{min} \le \frac{\mathbf{p}^T \mathbf{A} \mathbf{p}}{\|\mathbf{p}\|^2} \le \lambda_{max}$$

Eigenvector (Largest Eigenvalue)

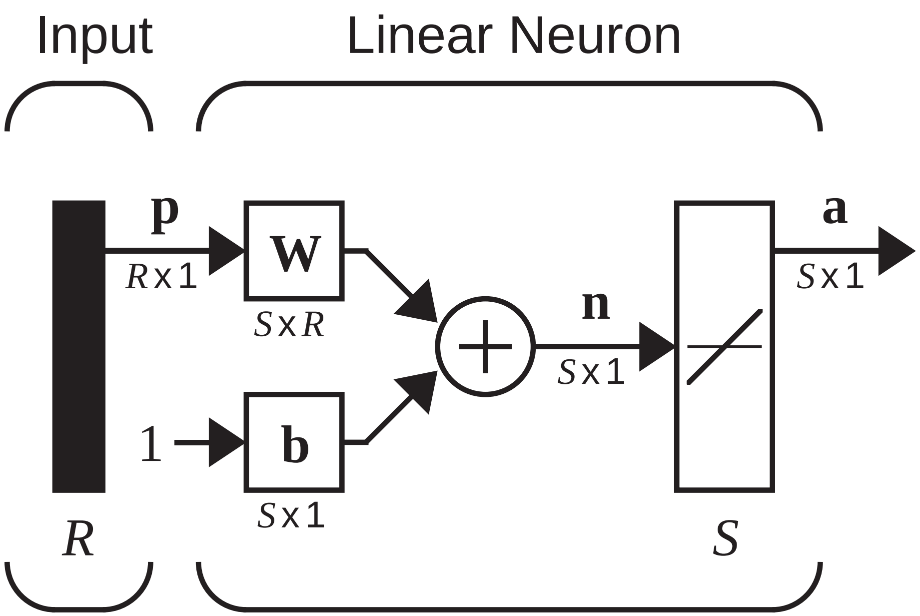
$$\mathbf{p} = \mathbf{z}_{max} \qquad\qquad \mathbf{c} = \mathbf{B}^T\mathbf{p} = \mathbf{B}^T\mathbf{z}_{max} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\frac{\mathbf{z}_{max}{}^T\mathbf{A}\mathbf{z}_{max}}{\|\mathbf{z}_{max}\|^2} = \frac{\sum_{i=1}^{n} \lambda_i c_i^2}{\sum_{i=1}^{n} c_i^2} = \lambda_{max}$$



The eigenvalues represent curvature (second derivatives) along the eigenvectors (the principal axes).

Linear Network



$$\mathbf{a} = \mathbf{purelin}(\mathbf{Wp}+\mathbf{b})$$

$$\mathbf{a} = \mathbf{purelin}(\mathbf{Wp}+\mathbf{b}) = \mathbf{Wp}+\mathbf{b}$$

$$a_i = purelin(n_i) = purelin({}_i\mathbf{w}^T\mathbf{p} + b_i) = {}_i\mathbf{w}^T\mathbf{p} + b_i$$

$${}_i\mathbf{w} = \begin{bmatrix} w_{i,1} \\ w_{i,2} \\ \vdots \\ w_{i,R} \end{bmatrix}$$

Performance Index

Training Set:

$$\{\mathbf{p}_1, \mathbf{t}_1\}, \{\mathbf{p}_2, \mathbf{t}_2\}, \ldots, \{\mathbf{p}_Q, \mathbf{t}_Q\}$$

Input: $\mathbf{p}_q$ Target: $\mathbf{t}_q$

Notation:

$$\mathbf{x} = \begin{bmatrix} {}_1\mathbf{w} \\ b \end{bmatrix} \qquad \mathbf{z} = \begin{bmatrix} \mathbf{p} \\ 1 \end{bmatrix} \qquad a = {}_1\mathbf{w}^T\mathbf{p} + b \Rightarrow a = \mathbf{x}^T\mathbf{z}$$

Mean Square Error:

$$F(\mathbf{x}) = E[e^2] = E[(t-a)^2] = E[(t-\mathbf{x}^T\mathbf{z})^2] = E_D$$

Error Analysis

$$F(\mathbf{x}) = E[e^2] = E[(t-a)^2] = E[(t-\mathbf{x}^T\mathbf{z})^2]$$

$$F(\mathbf{x}) = E[t^2 - 2t\mathbf{x}^T\mathbf{z} + \mathbf{x}^T\mathbf{z}\mathbf{z}^T\mathbf{x}]$$

$$F(\mathbf{x}) = E[t^2] - 2\mathbf{x}^T \mathrm{E}[t\mathbf{z}] + \mathbf{x}^T E[\mathbf{z}\mathbf{z}^T]\mathbf{x}$$

$$\boxed{F(\mathbf{x}) = c - 2\mathbf{x}^T\mathbf{h} + \mathbf{x}^T\mathbf{R}\mathbf{x}}$$

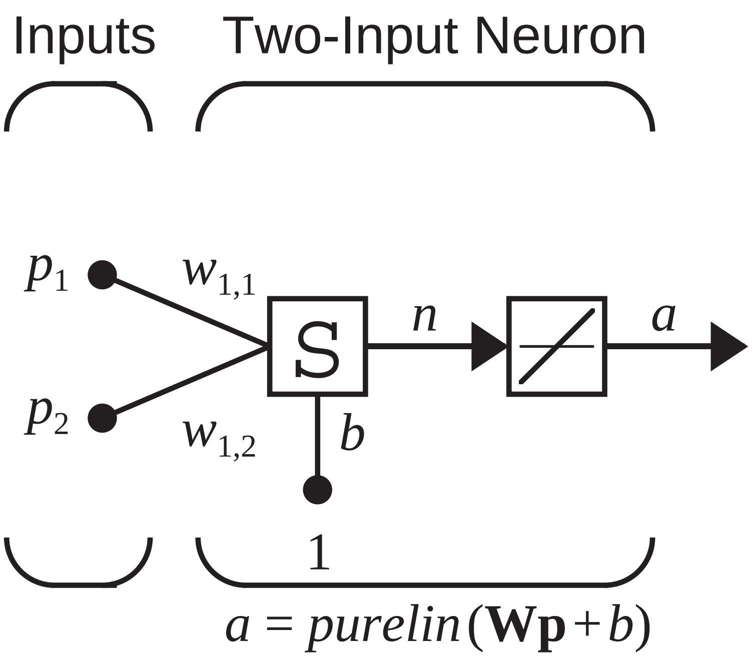
$$c = E[t^2] \qquad \mathbf{h} = E[t\mathbf{z}] \qquad \mathbf{R} = E[\mathbf{z}\mathbf{z}^T]$$

The mean square error for the Linear Network is a quadratic function:

$$F(\mathbf{x}) = c + \mathbf{d}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}$$

$$\mathbf{d} = -2\mathbf{h} \qquad \mathbf{A} = 2\mathbf{R}$$

Example



$$\left\{\mathbf{p}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, t_1 = 1\right\} \quad \text{(Probability = 0.75)}$$

$$\left\{\mathbf{p}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}, t_2 = -1\right\} \quad \text{(Probability = 0.25)}$$

$$F(\mathbf{x}) = c - 2\mathbf{x}^T\mathbf{h} + \mathbf{x}^T\mathbf{R}\mathbf{x} = E_D$$

$$c = E[t^2] = (1)^2(0.75) + (-1)^2(0.25) = 1$$

$$\mathbf{h} = E[t\mathbf{z}] = (0.75)(1)\begin{bmatrix} 1 \\ 1 \end{bmatrix} + (0.25)(-1)\begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}$$

$$\mathbf{R} = E[\mathbf{z}\mathbf{z}^T] = \mathbf{p}_1\mathbf{p}_1^T(0.75) + \mathbf{p}_2\mathbf{p}_2^T(0.25)$$

$$= 0.75\begin{bmatrix} 1 \\ 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \end{bmatrix} + 0.25\begin{bmatrix} -1 \\ 1 \end{bmatrix}\begin{bmatrix} -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

Performance Contour

Optimum Point (Maximum Likelihood)

$$\mathbf{x}^{ML} = -\mathbf{A}^{-1}\mathbf{d} = \mathbf{R}^{-1}\mathbf{h} = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Hessian Matrix

$$\nabla^2 F(\mathbf{x}) = \mathbf{A} = 2\mathbf{R} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

Eigenvalues

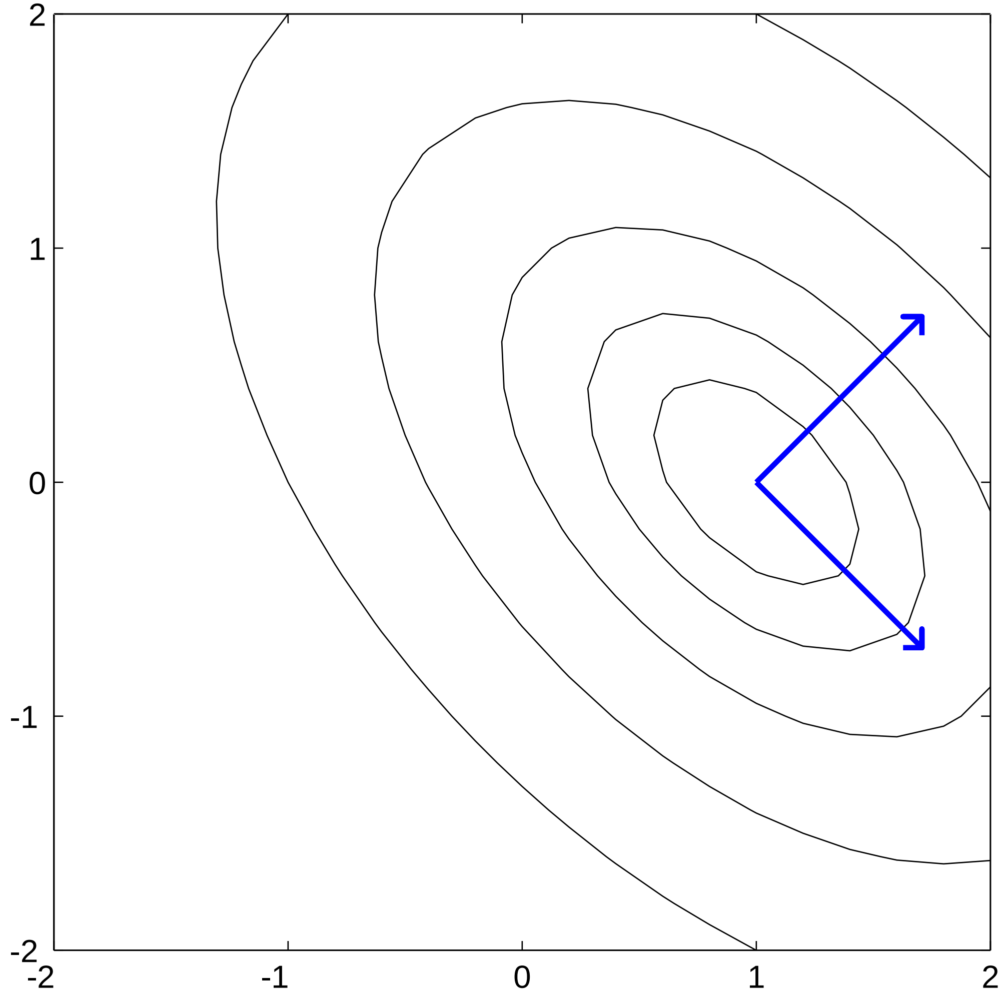
$$\left| \mathbf{A} - \lambda \mathbf{I} \right| = \begin{vmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{vmatrix} = \lambda^2 - 4\lambda + 3 = (\lambda - 1)(\lambda - 3) \Rightarrow \lambda_1 = 1, \qquad \lambda_2 = 3$$

Eigenvectors

$$\left[\mathbf{A} - \lambda \mathbf{I}\right]\mathbf{v} = 0$$

$$\lambda_1 = 1 \qquad \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\mathbf{v}_1 = 0 \qquad \mathbf{v}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad \lambda_2 = 3 \qquad \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}\mathbf{v}_2 = 0 \qquad \mathbf{v}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Contour Plot of E_D



$$\gamma = N - 2\alpha^{\mathrm{MP}} \mathrm{tr}(\mathbf{H}^{\mathrm{MP}})^{-1}$$

Steepest Descent Trajectory

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha\mathbf{g}_k = \mathbf{x}_k - \alpha(\mathbf{A}\mathbf{x}_k + \mathbf{d})$$

$$= \mathbf{x}_k - \alpha\mathbf{A}(\mathbf{x}_k + \mathbf{A}^{-1}\mathbf{d}) = \mathbf{x}_k - \alpha\mathbf{A}(\mathbf{x}_k - \mathbf{x}^{ML})$$

$$= [\mathbf{I} - \alpha\mathbf{A}]\mathbf{x}_k + \alpha\mathbf{A}\mathbf{x}^{ML} = \mathbf{M}\mathbf{x}_k + [\mathbf{I} - \mathbf{M}]\mathbf{x}^{ML}$$

$$\boxed{\mathbf{M} = [\mathbf{I} - \alpha\mathbf{A}]}$$

$$\mathbf{x}_1 = \mathbf{M}\mathbf{x}_0 + [\mathbf{I} - \mathbf{M}]\mathbf{x}^{ML}$$

$$\mathbf{x}_2 = \mathbf{M}\mathbf{x}_1 + [\mathbf{I} - \mathbf{M}]\mathbf{x}^{ML}$$

$$= \mathbf{M}^2\mathbf{x}_0 + \mathbf{M}[\mathbf{I} - \mathbf{M}]\mathbf{x}^{ML} + [\mathbf{I} - \mathbf{M}]\mathbf{x}^{ML}$$

$$= \mathbf{M}^2\mathbf{x}_0 + \mathbf{M}\mathbf{x}^{ML} - \mathbf{M}^2\mathbf{x}^{ML} + \mathbf{x}^{ML} - \mathbf{M}\mathbf{x}^{ML}$$

$$= \mathbf{M}^2\mathbf{x}_0 + \mathbf{x}^{ML} - \mathbf{M}^2\mathbf{x}^{ML} = \mathbf{M}^2\mathbf{x}_0 + [\mathbf{I} - \mathbf{M}^2]\mathbf{x}^{ML}$$

$$\boxed{\mathbf{x}_k = \mathbf{M}^k\mathbf{x}_0 + [\mathbf{I} - \mathbf{M}^k]\mathbf{x}^{ML}}$$

Regularization

$$F(\mathbf{x}) = E_D + \gamma E_W \qquad (\gamma = \alpha/\beta)$$

$$E_W = \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0)$$

To locate the minimum point, set the gradient to zero.

$$\nabla F(\mathbf{x}) = \nabla E_D + \gamma \nabla E_W$$

$$\nabla E_W = (\mathbf{x} - \mathbf{x}_0) \qquad \nabla E_D = \mathbf{A}(\mathbf{x} - \mathbf{x}^{ML})$$

$$\nabla F(\mathbf{x}) = \mathbf{A}(\mathbf{x} - \mathbf{x}^{ML}) + \gamma(\mathbf{x} - \mathbf{x}_0) = \mathbf{0}$$

MAP – ML

$$\mathbf{A}(\mathbf{x}^{MAP} - \mathbf{x}^{ML}) = -\gamma(\mathbf{x}^{MAP} - \mathbf{x}_0) = -\gamma(\mathbf{x}^{MAP} - \mathbf{x}^{ML} + \mathbf{x}^{ML} - \mathbf{x}_0)$$

$$= -\gamma(\mathbf{x}^{MAP} - \mathbf{x}^{ML}) - \gamma(\mathbf{x}^{ML} - \mathbf{x}_0)$$

$$(\mathbf{A} + \gamma\mathbf{I})(\mathbf{x}^{MAP} - \mathbf{x}^{ML}) = \gamma(\mathbf{x}_0 - \mathbf{x}^{ML})$$

$$(\mathbf{x}^{MAP} - \mathbf{x}^{ML}) = \gamma(\mathbf{A} + \gamma\mathbf{I})^{-1}(\mathbf{x}_0 - \mathbf{x}^{ML})$$

$$\mathbf{x}^{MAP} = \mathbf{x}^{ML} - \gamma(\mathbf{A} + \gamma\mathbf{I})^{-1}\mathbf{x}^{ML} + \gamma(\mathbf{A} + \gamma\mathbf{I})^{-1}\mathbf{x}_0 = \mathbf{x}^{ML} - \mathbf{M}_\gamma\mathbf{x}^{ML} + \mathbf{M}_\gamma\mathbf{x}_0$$

$$\mathbf{M}_\gamma = \gamma(\mathbf{A} + \gamma\mathbf{I})^{-1}$$

$$\boxed{\mathbf{x}^{MAP} = \mathbf{M}_\gamma\mathbf{x}_0 + [\mathbf{I} - \mathbf{M}_\gamma]\mathbf{x}^{ML}}$$

Early Stopping – Regularization

$$\mathbf{x}_k = \mathbf{M}^k \mathbf{x}_0 + [\mathbf{I} - \mathbf{M}^k]\mathbf{x}^{ML}$$

$$\mathbf{x}^{MAP} = \mathbf{M}_\gamma \mathbf{x}_0 + [\mathbf{I} - \mathbf{M}_\gamma]\mathbf{x}^{ML}$$

$$\mathbf{M} = [\mathbf{I} - \alpha\mathbf{A}]$$

$$\mathbf{M}_\gamma = \gamma(\mathbf{A} + \gamma\mathbf{I})^{-1}$$

Eigenvalues of $\mathbf{M}^k$:

$$[\mathbf{I} - \alpha\mathbf{A}]\mathbf{z}_i = \mathbf{z}_i - \alpha\mathbf{A}\mathbf{z}_i = \mathbf{z}_i - \alpha\lambda_i\mathbf{z}_i = \underbrace{(1 - \alpha\lambda_i)}_{\text{Eigenvalues of } \mathbf{M}}\mathbf{z}_i$$

$\mathbf{z}_i$ - eigenvector of $\mathbf{A}$

λ_i - eigenvalue of $\mathbf{A}$

$$\mathrm{eig}(\mathbf{M}^k) = (1 - \alpha\lambda_i)^k$$

Eigenvalues of $\mathbf{M}_\gamma$:

$$\mathrm{eig}(\mathbf{M}_\gamma) = \frac{\gamma}{(\lambda_\mathrm{i} + \gamma)}$$

Reg. Parameter – Iteration Number

$\mathbf{M}^k$ and $\mathbf{M}_\gamma$ have the same eigenvectors. They would be equal if their eigenvalues were equal.

$$\frac{\gamma}{(\lambda_i + \gamma)} = (1 - \alpha\lambda_i)^k \qquad \text{Taking log :} \qquad -\log\left(1 + \frac{\lambda_i}{\gamma}\right) = k\log(1 - \alpha\lambda_i)$$

Since these are equal at $\lambda_i = 0$, they are always equal if the slopes are equal.

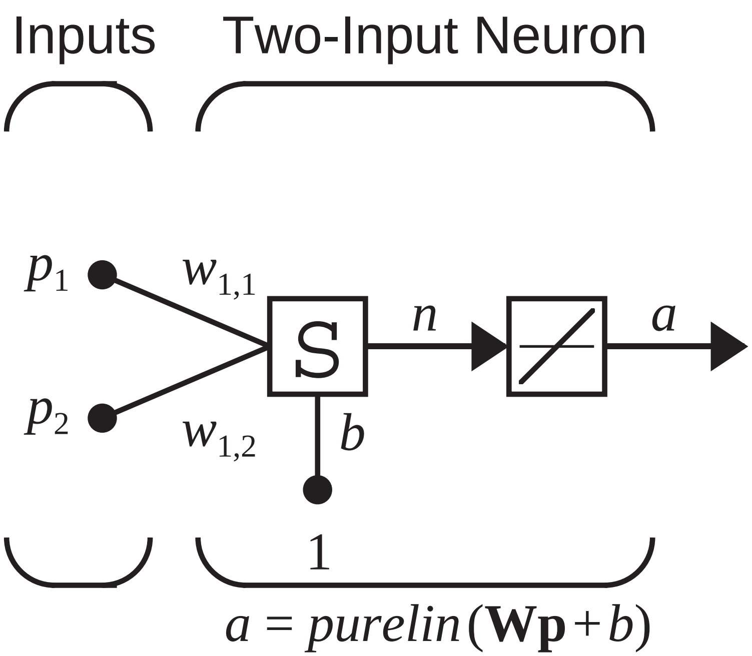
$$-\frac{1}{\left(1 + \frac{\lambda_i}{\gamma}\right)}\frac{1}{\gamma} = \frac{k}{1 - \alpha\lambda_i}(-\alpha) \quad \Longrightarrow \quad \alpha k = \frac{1}{\gamma}\,\frac{(1 - \alpha\lambda_i)}{(1 + \lambda_i/\gamma)}$$

If $\alpha\lambda_i$ and λ_i/γ are small, then:

$$\boxed{\alpha k \cong \frac{1}{\gamma}}$$

(Increasing the number of iterations is equivalent to decreasing the regularization parameter!)

Example



$$\left\{\mathbf{p}_1 = \begin{bmatrix}1\\1\end{bmatrix}, t_1 = 1\right\}$$ (Probability = 0.75)

$$\left\{\mathbf{p}_2 = \begin{bmatrix}-1\\1\end{bmatrix}, t_2 = -1\right\}$$ (Probability = 0.25)

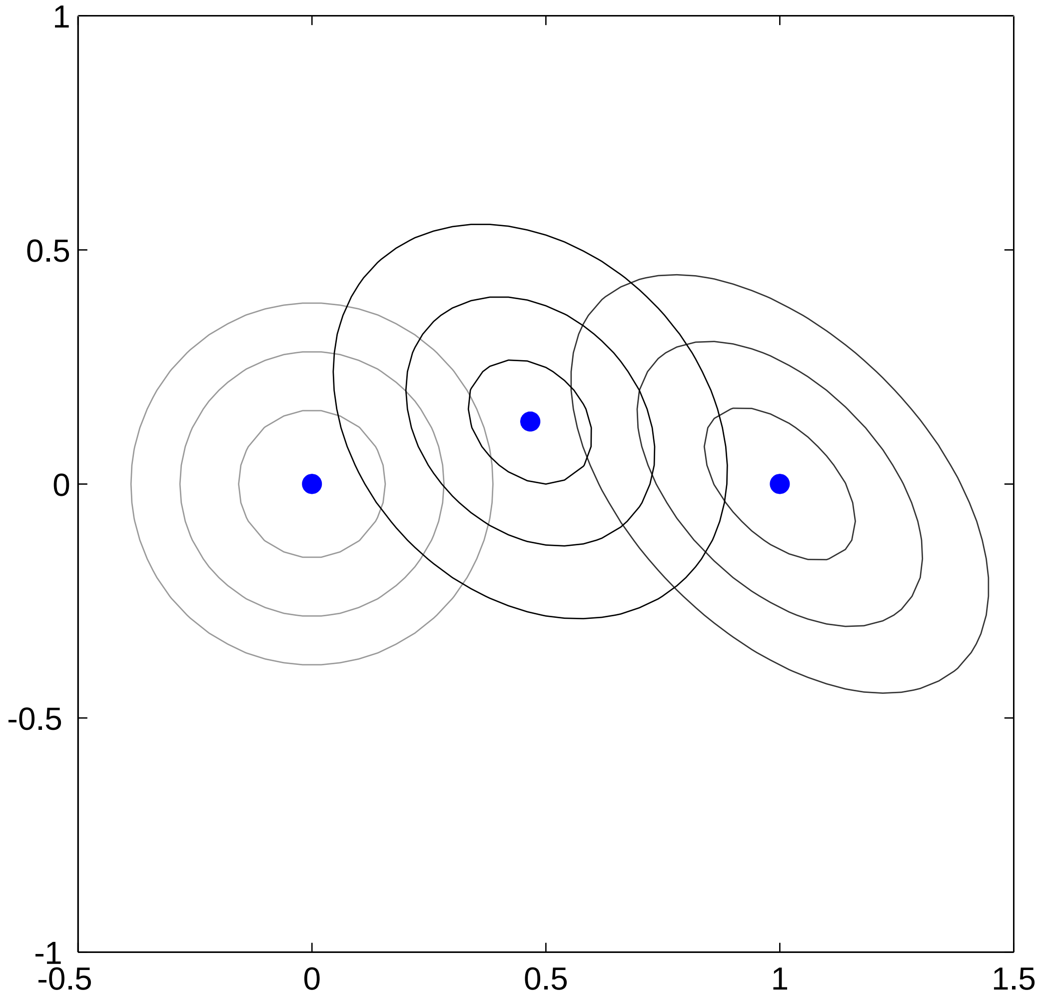
$$F(\mathbf{x}) = E_D + \gamma E_W$$

$$E_D = c + \mathbf{x}^T\mathbf{d} + \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}$$

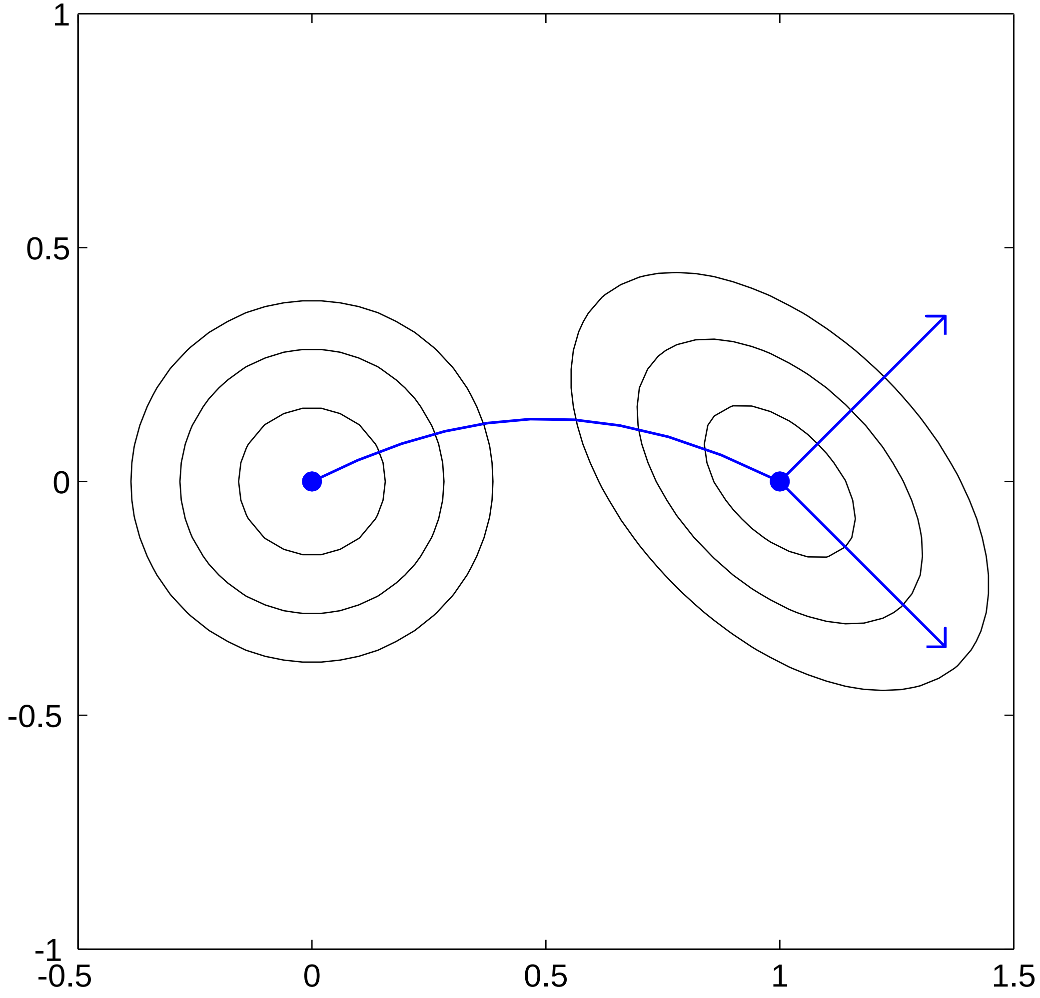
$$E_W = \frac{1}{2}\mathbf{x}^T\mathbf{x} \qquad c = 1 \qquad \mathbf{d} = -2\mathbf{h} = \begin{bmatrix}-2\\-1\end{bmatrix} \qquad \mathbf{A} = 2\mathbf{R} = \begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}$$

$$\nabla^2 F(\mathbf{x}) = \nabla^2 E_D + \gamma\nabla^2 E_W = \begin{bmatrix}2 & 1\\1 & 2\end{bmatrix} + \gamma\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} = \begin{bmatrix}2+\gamma & 1\\1 & 2+\gamma\end{bmatrix}$$

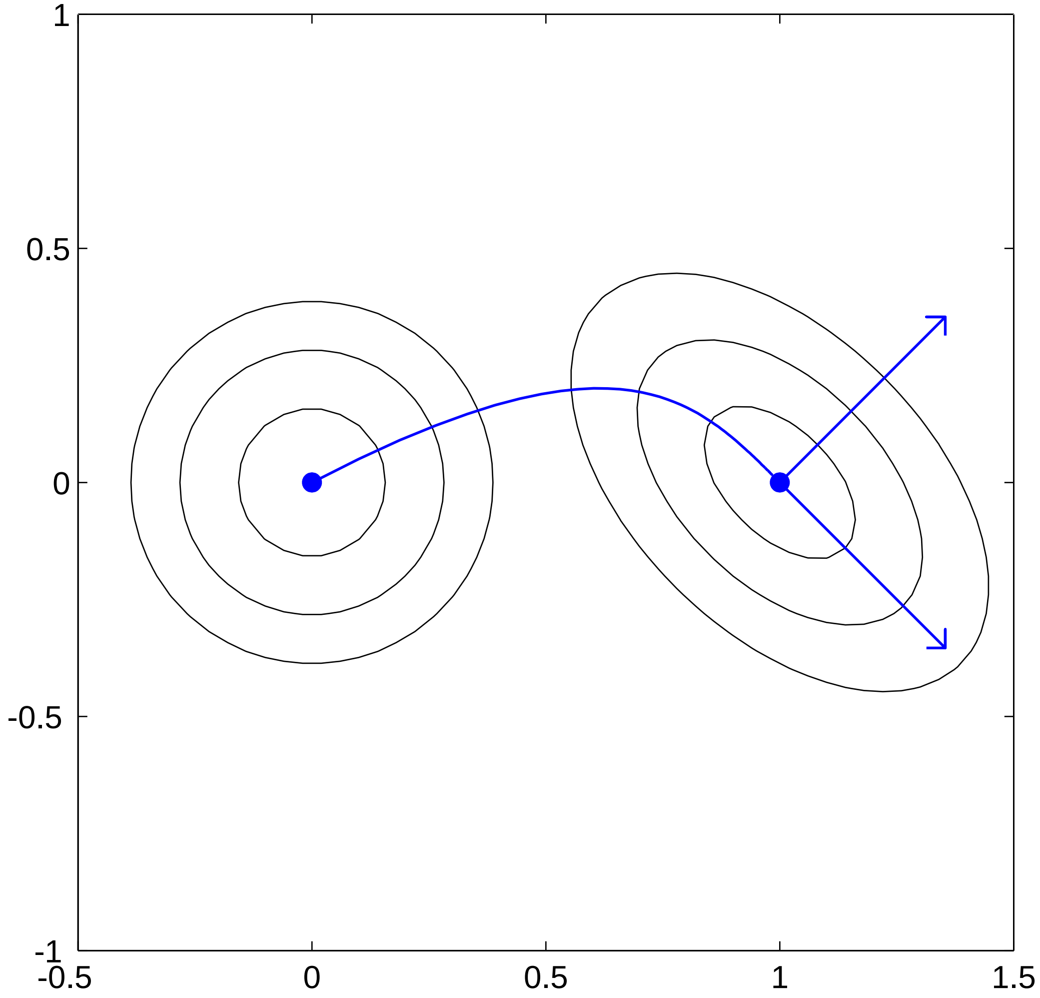
$\gamma = 0, 2, \infty$



$\gamma = 0 \to \infty$



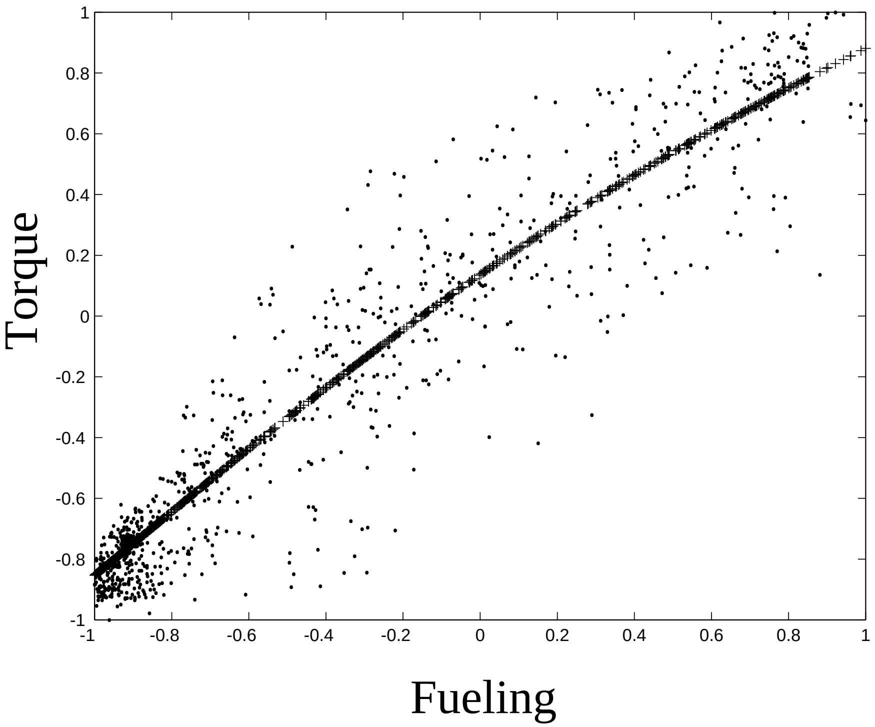
Steepest Descent Path



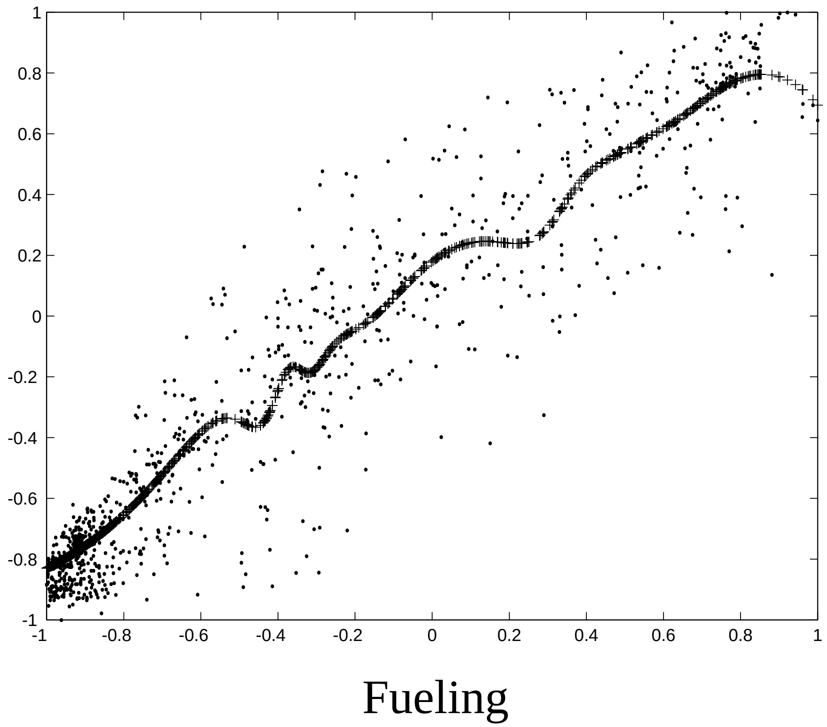
Engine Fueling-Torque

1-10-1 Network

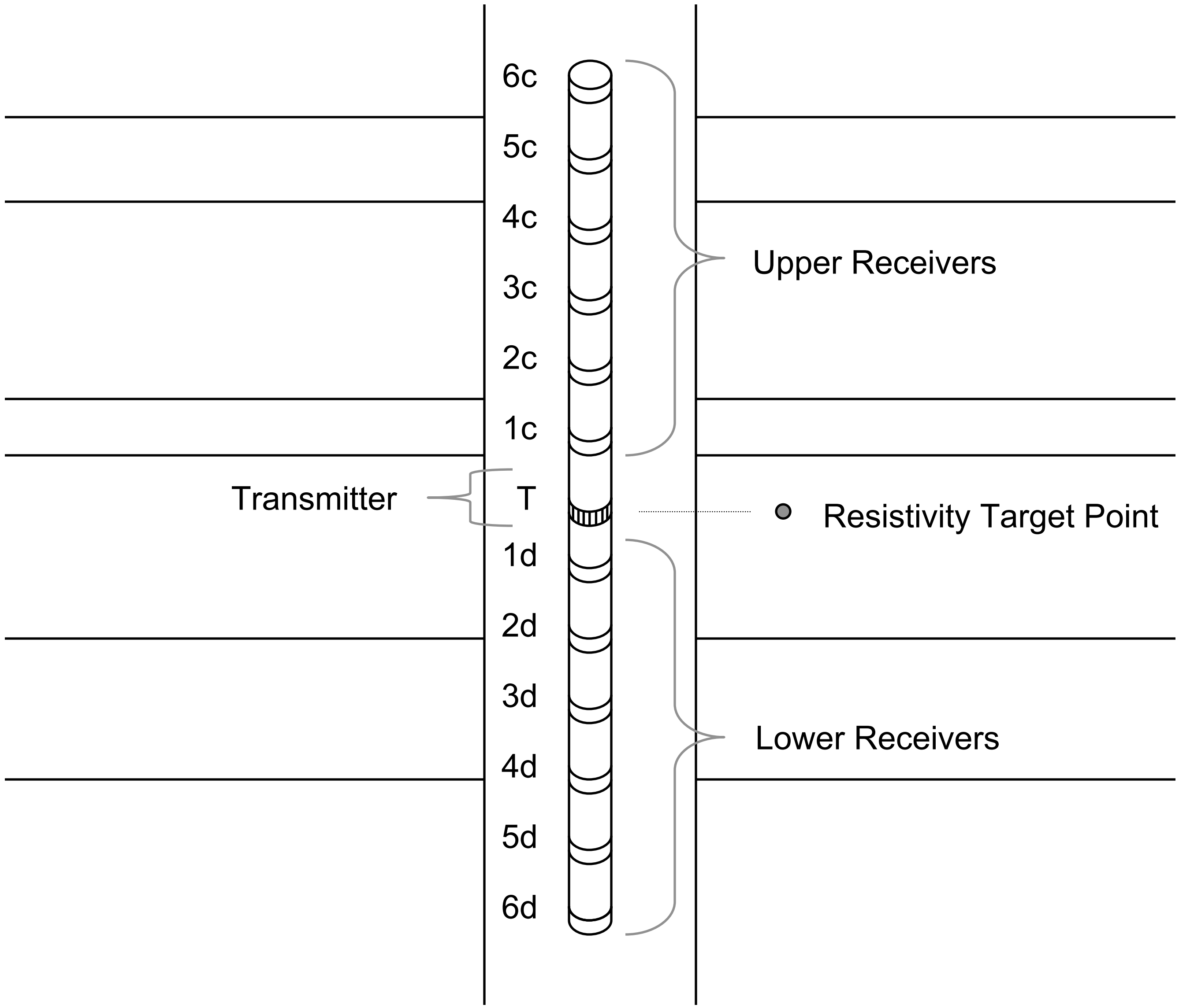
Using Bayesian Regularization



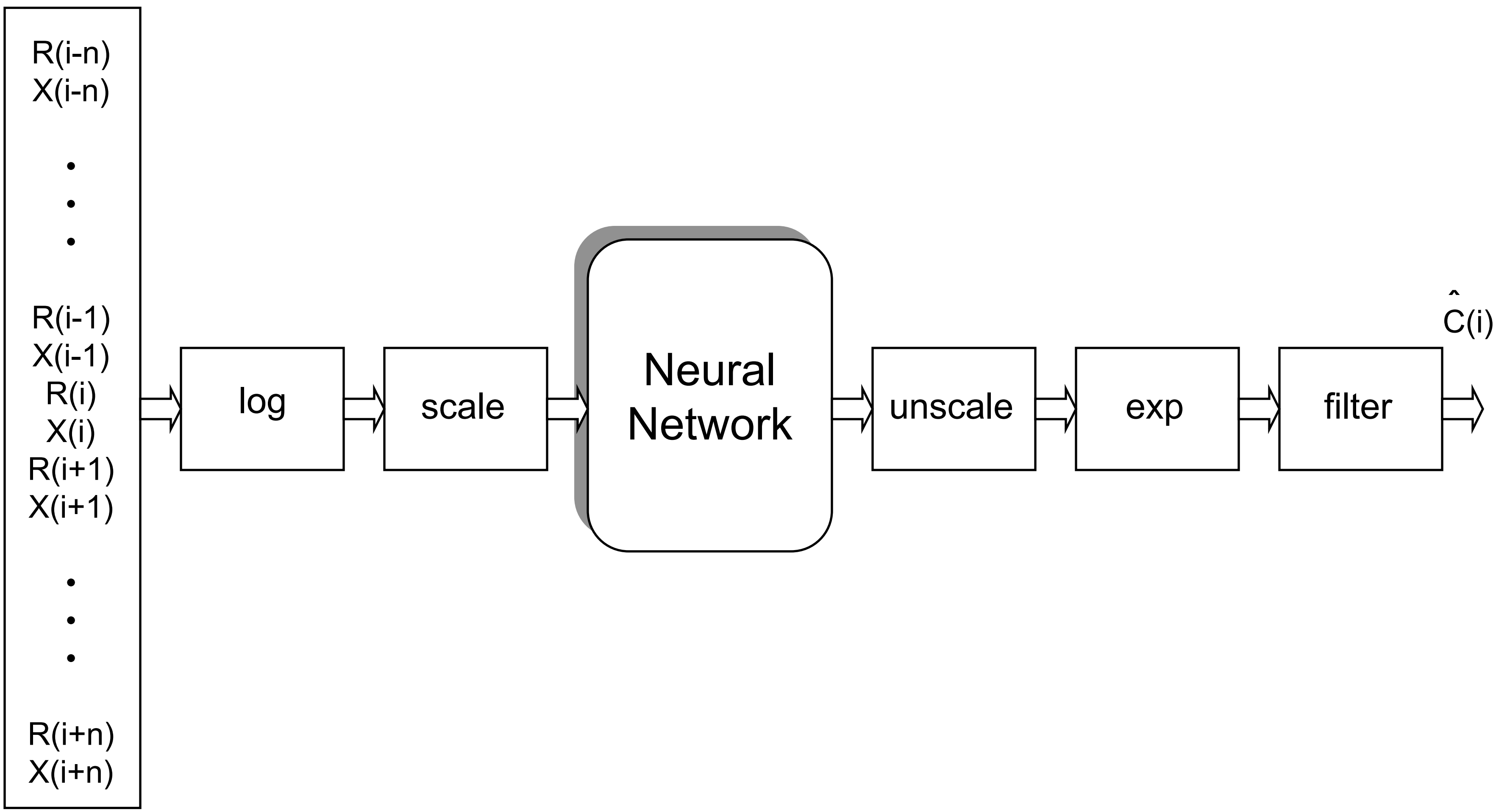
Using Early Stopping



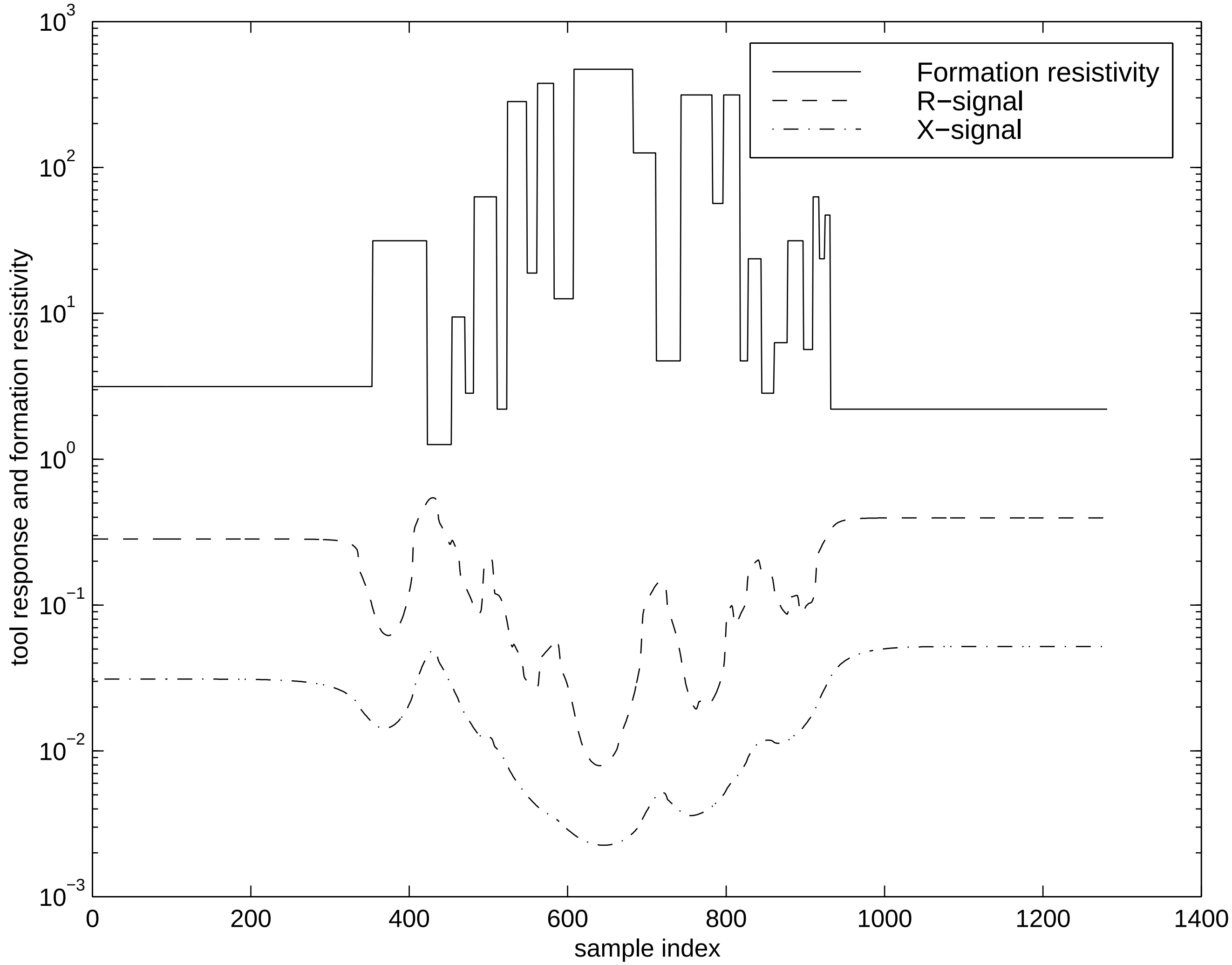
Induction Tool



Typical Filter Structure

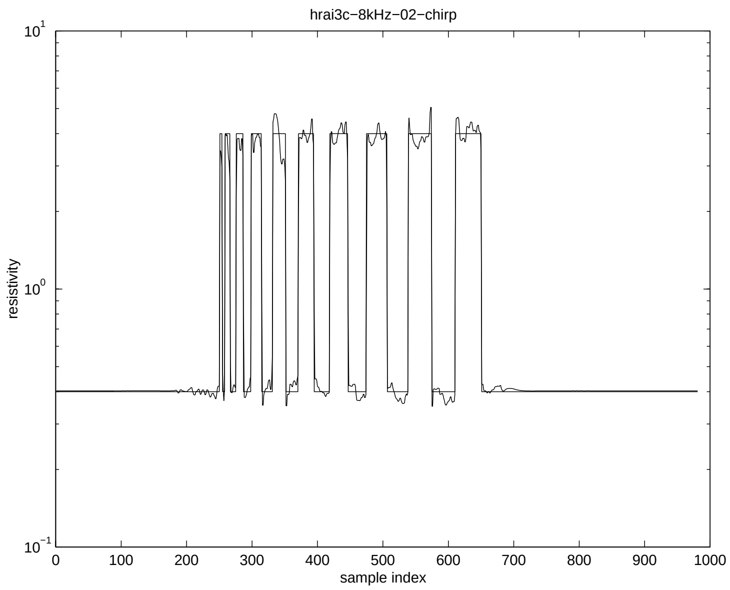


Typical Tool Response

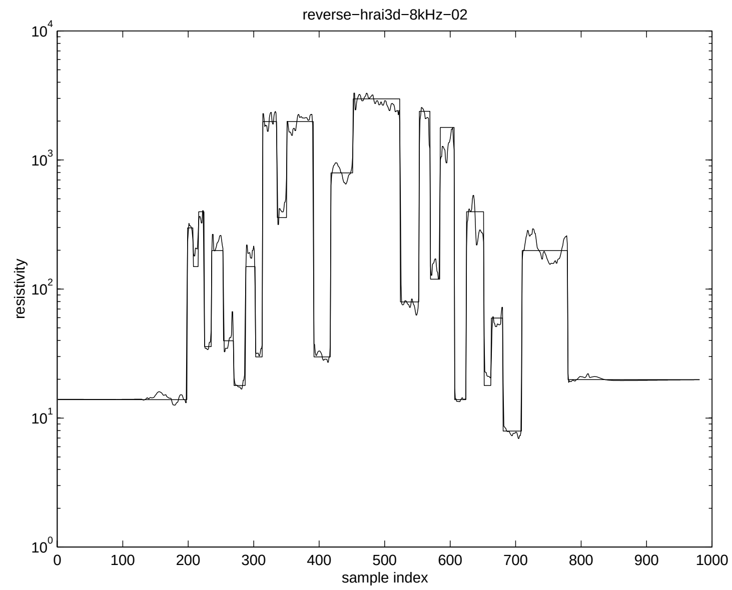


Prediction Results

D2 Testing Subset



RD1 Testing Subset



Summary

- Regularization improves generalization.
- Bayesian framework is attractive.
- Regularization and early stopping are approximately equivalent processes.
- When using early stopping a relatively slow training algorithm should be used.
- Increasing the length of training is equivalent to reducing the regularization.
- The effective number of parameters increases during the training process.
- Regularization usually produces a “smoother” function.

References

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