Linear Regression

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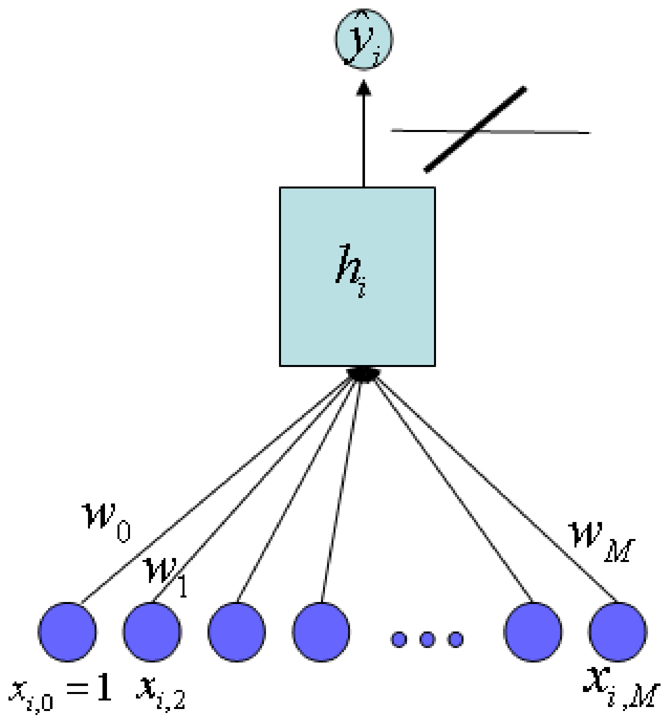
Learning Machine: The Linear Model / ADALINE



- As with the Perceptron we start with an activation functions that is a linearly weighted sum of the inputs

$$h_i = \sum_{j=0}^{M-1} w_{i,j} x_{i,j}$$

(Note: $x_{i,0} = 1$ is a constant input, so that w_0 is the bias)

- The activation is the the output (no thresholding)

$$\hat{y}_i = f(\mathbf{x}_i) = h_i$$

- Regression: when the target function can take on real values

Method of Least Squares

- Squared-loss cost function:

$$\text{cost}(\mathbf{w}) = \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

- The parameters that minimize the cost function are called least squares (LS) estimators

$$\mathbf{w}_{ls} = \arg\min_{w} \text{cost}(\mathbf{w})$$

- For visualization, on chooses $M = 2$ (although linear regression is often applied to high-dimensional inputs)

Least-squares Estimator for Regression

One-dimensional regression:

$$f(x, \mathbf{w}) = w_0 + w_1 x$$

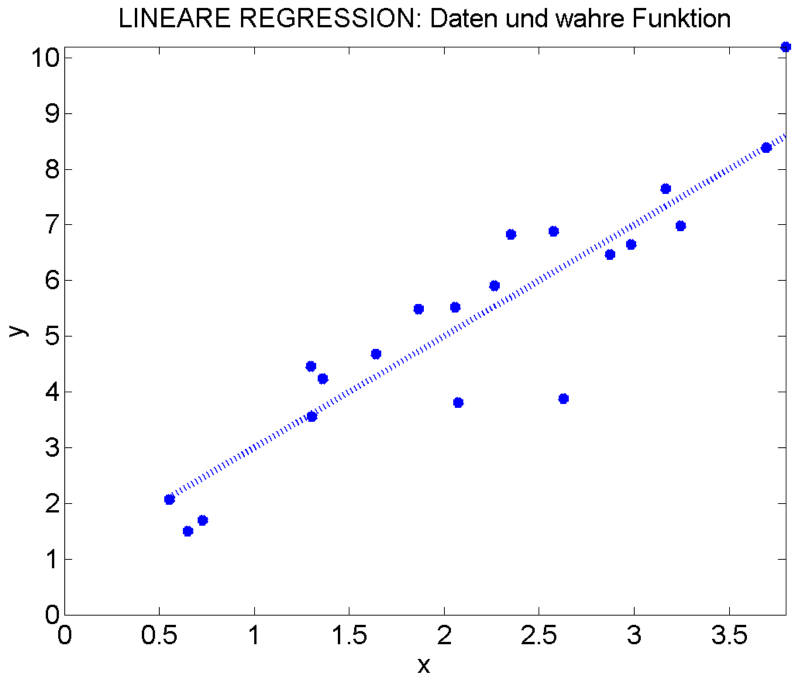
$$\mathbf{w} = (w_0, w_1)^T$$

Squared error:

$$\text{cost}(\mathbf{w}) = \sum_{i=1}^{N} (y_i - f(x_i, \mathbf{w}))^2$$

Goal:

$$\mathbf{w}_{ls} = \arg\min_{w} \text{cost}(\mathbf{w})$$



$$w_0 = 1, w_1 = 2, var(\epsilon) = 1$$

Least-squares Estimator in General

General Model:

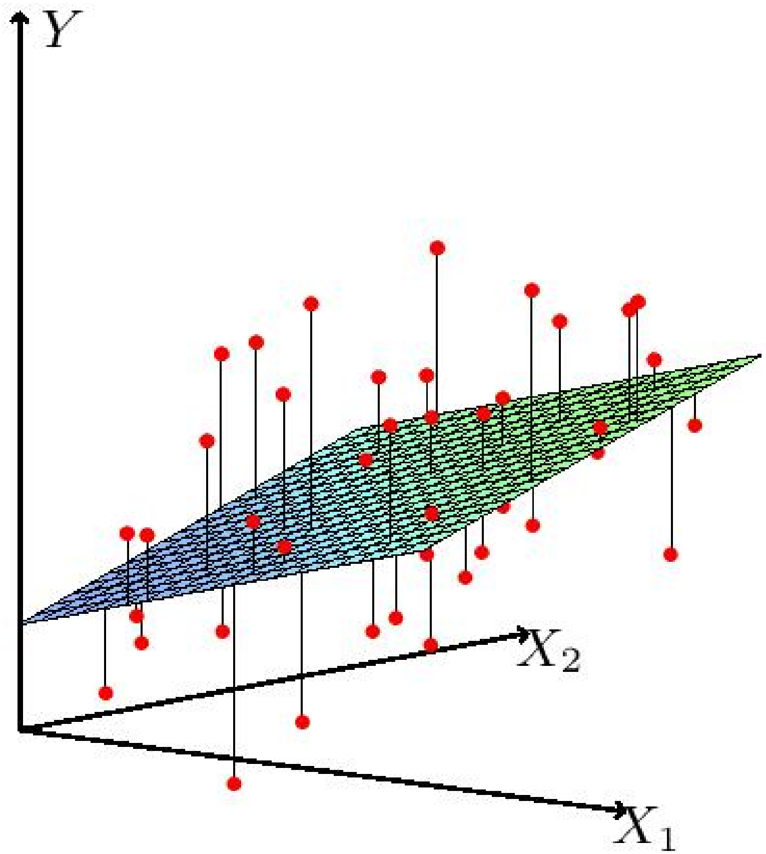
$$f(\mathbf{x}_i, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j x_{i,j}$$

$$= \mathbf{x}_i^T \mathbf{w}$$

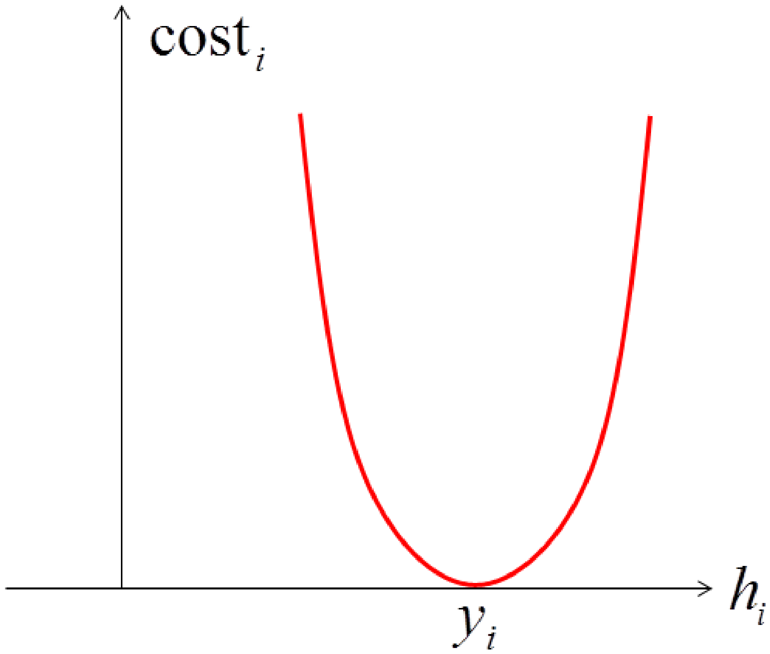
$$\mathbf{w} = (w_0, w_1, \ldots w_{M-1})^T$$

$$\mathbf{x}_i = (1, x_{i,1}, \ldots, x_{i,M-1})^T$$

Linear Regression with Several Inputs



Contribution to the Cost Function of one Data Point



Gradient Descent Learning

- Initialize parameters (typically using small random numbers)
- Adapt the parameters in the direction of the negative gradient
- With

$$\text{cost}(\mathbf{w}) = \sum_{i=1}^{N} \left(y_i - \sum_{j=0}^{M-1} w_j x_{i,j} \right)^2$$

- The parameter gradient is (Example: w_j)

$$\frac{\partial \text{cost}}{\partial w_j} = -2 \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i)) x_{i,j}$$

- A sensible learning rule is

$$w_j \longleftarrow w_j + \eta \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i)) x_{i,j}$$

ADALINE-Learning Rule

- ADALINE: ADAptive LINear Element
- The ADALINE uses stochastic gradient descent (SGE)
- Let $\mathbf{x}_t$ and y_t be the training pattern in iteration t. The we adapt, $t = 1, 2, \ldots$

$$w_j \longleftarrow w_j + \eta(y_t - \hat{y}_t)x_{t,j} \quad j = 1, 2, \ldots, M$$

- $\eta > 0$ is the learning rate, typically $0 < \eta << 0.1$
- Compare: the Perceptron learning rule (only applied to misclassified patterns)

$$w_j \longleftarrow w_j + \eta y_t x_{t,j} \quad j = 1, \ldots, M$$

Analytic Solution

- The least-squares solution can be calculated in one step

Cost Function in Matrix Form

$$\text{cost}(\mathbf{w}) = \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

$$= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$\mathbf{y} = (y_1, \ldots, y_N)^T$$

$$\mathbf{X} = \begin{pmatrix} x_{1,0} & \cdots & x_{1,M-1} \\ \cdots & \cdots & \cdots \\ x_{N,0} & \cdots & x_{N,M-1} \end{pmatrix}$$

Calculating the First Derivative

Matrix calculus:

$\mathbf{y}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$
$\mathbf{A}\mathbf{x}$	$\mathbf{A}^T$
$\mathbf{x}^T\mathbf{A}$	$\mathbf{A}$
$\mathbf{x}^T\mathbf{x}$	$2\mathbf{x}$
$\mathbf{x}^T\mathbf{A}\mathbf{x}$	$\mathbf{A}\mathbf{x} + \mathbf{A}^T\mathbf{x}$

Thus

$$\frac{\partial \text{cost}(\mathbf{w})}{\partial \mathbf{w}} = \frac{\partial(\mathbf{y} - \mathbf{X}\mathbf{w})}{\partial w} \times 2(\mathbf{y} - \mathbf{X}\mathbf{w}) = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

Setting First Derivative to Zero

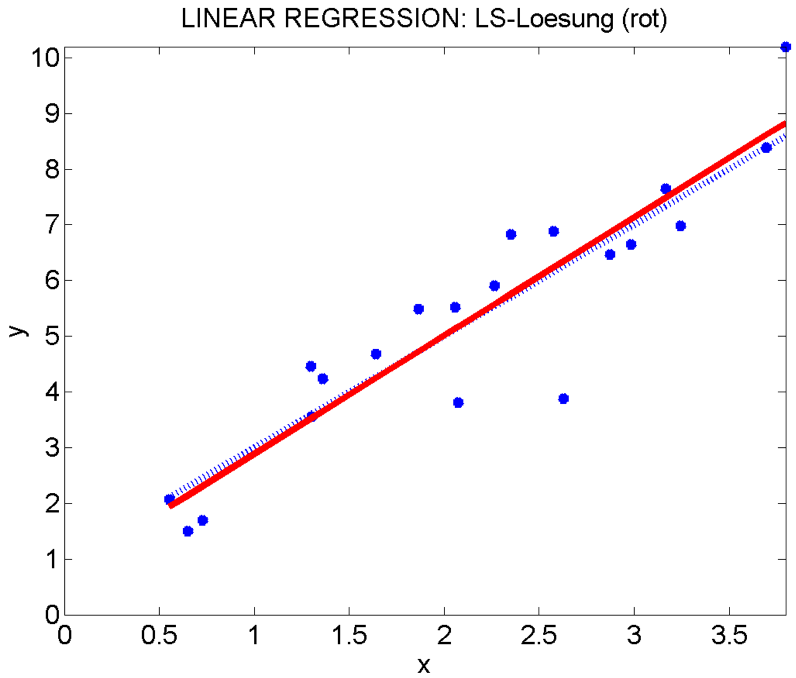
Calculating the LS-solution:

$$\frac{\partial \text{cost}(\mathbf{w})}{\partial \mathbf{w}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) = 0$$

$$\hat{\mathbf{w}}_{ls} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Complexity (linear in N!):

$$\mathcal{O}(M^3 + NM^2)$$



$$\hat{w}_0 = 0.75, \hat{w}_1 = 2.13$$

Stability of the Solution

- When $N >> M$, the LS solution is stable (small changes in the data lead to small changes in the paramater estimates)
- When $N < M$ then there are many solutions which all produce the zero training error
- Of all these solutions, one selects the one that minimizes $\sum_{i=0}^{M} w_i^2$ (regularised solution)
- Even with $N > M$ it is advantageous to regularize the solution, in particular with noise on the target

Linear Regression and Regularisation

- Regularised cost function (*Penalized Least Squares* (PLS), *Ridge Regression*, *Weight Decay*): the influence of a single data point should be small

$$\text{cost}^{pen}(\mathbf{w}) = \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i, \mathbf{w}))^2 + \lambda \sum_{i=0}^{M-1} w_i^2$$

$$\hat{\mathbf{w}}_{pen} = \left(\mathbf{X}^T\mathbf{X} + \lambda I\right)^{-1} \mathbf{X}^T\mathbf{y}$$

Derivation:

$$\frac{\partial J_N^{pen}(\mathbf{w})}{\partial \mathbf{w}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) + 2\lambda\mathbf{w} = 2[-\mathbf{X}^T\mathbf{y} + (\mathbf{X}^T\mathbf{X} + \lambda I)\mathbf{w}]$$

Example

- Three data points are generated as (true model)

$$y_i = 0.5 + x_{i,1} + \epsilon_i$$

  Here, ϵ_i is independent noise

- (correct) model 1

$$f(\mathbf{x}_i) = w_0 + w_1 x_{i,1}$$

- Training data for model 1:

x_1	y
-0.2	0.49
0.2	0.64
1	1.39

- The LS solution gives $\mathbf{w}_{ls} = (0.58, 0.77)$
- In comparison,the true parameters are: $\mathbf{w} = (0.50, 1.00)$

Model 2

- Here we generate a second correlated input

$$x_{i,2} = x_{i,1} + \delta_i$$

  Again, δ_i is uncorrelated noise

- Modell 2

$$f(\mathbf{x}_i) = w_0 + w_1 x_{i,1} + w_2 x_{i,2}$$

  Daten, die Modell 2 sieht:

x_1	x_2	y
-0.2	-0.1996	0.49
0.2	0.1993	0.64
1	1.0017	1.39

- Die least squares solution gives $\mathbf{w}_{ls} = (0.67, -136, 137)$!!!

Model 2 with Regularisation

- All as before, only that large weights are penalized
- Die penalized least squares solution gives $\mathbf{w}_{pen} = (0.58, 0.38, 0.39)$!!!
- Compare: the LS-solution for model-2 gave $\mathbf{w}_{ls} = (0.58, 0.77)$
- The collinearity (strong correlation of the inputs) hurts the LS-solution but does not hurt the penalized LS solution. We even obtain a higher robustness with respect to errors in the inputs, since weights are smaller!

Training Data

- Training:

y	$M1 : \widehat{y}_{ML}$	$M2 : \widehat{y}_{ML}$	$M2 : \widehat{y}_{pen}$
0.50	0.43	0.50	0.43
0.65	0.74	0.65	0.74
1.39	1.36	1.39	1.36

- For Model 1 and Model 2 with regularization we have nonzero error on the training data
- For Model 2 without regularization, the training error is zero
- If we only consider the training error, we would prefer Model 2

Test Data

- Test Data:

y	$M1 : \widehat{y}_{ML}$	$M2 : \widehat{y}_{ML}$	$M2 : \widehat{y}_{pen}$
0.20	0.36	0.69	0.36
0.80	0.82	0.51	0.82
1.10	1.05	1.30	1.05

- On test data model 1 and model 2 with regularization give better results

- Even more dramatic: extrapolation

Experiments with real world data: data from Prostate Cancer

8 Inputs, 97 data points; y: Prostate-specific antigen

	LS	0.586
10-times cross validation	Best Subset (3)	0.574
	Ridge (Weight Decay)	0.540

GWAS Study

Correlation with disease (systemic sclerosis) versus location of SNPs on the gene. The regression weight of a single SNP as an input is calculated with other inputs representing general personal traits (male/femal, Caucasian, Asian, PCA features, ...). Repeated for all SNPs (maybe 1 Mio).