Linear Regression

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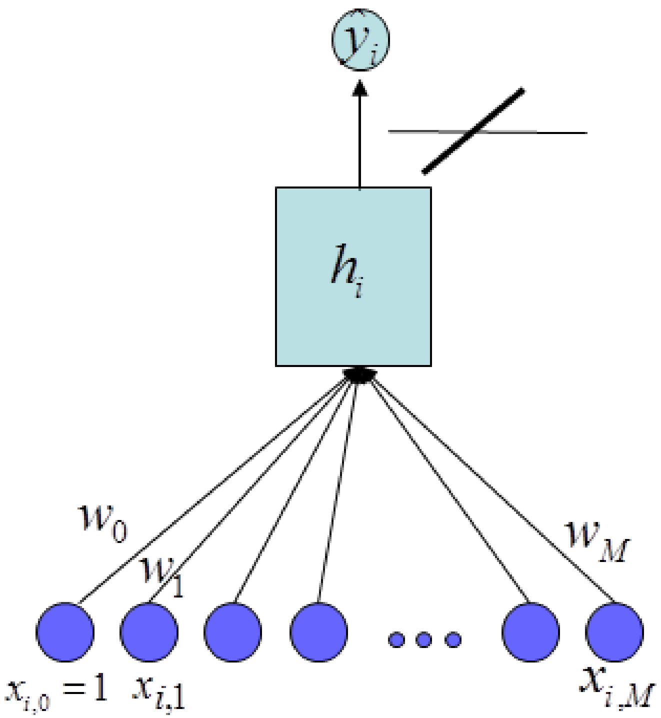
2016

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

$$h = \sum_{j=0}^{M-1} w_j x_j$$

(Note: $x_0 = 1$ is a constant input, so that w_0 is the bias)

- New: **The activation is the output** (no thresholding)

$$\hat{y} = f_{\mathbf{w}}(\mathbf{x}) = h$$

- Regression: the target function can take on real values

Method of Least Squares

- Squared-loss cost function:

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

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

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

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

Least-squares Estimator for Regression

One-dimensional regression:

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

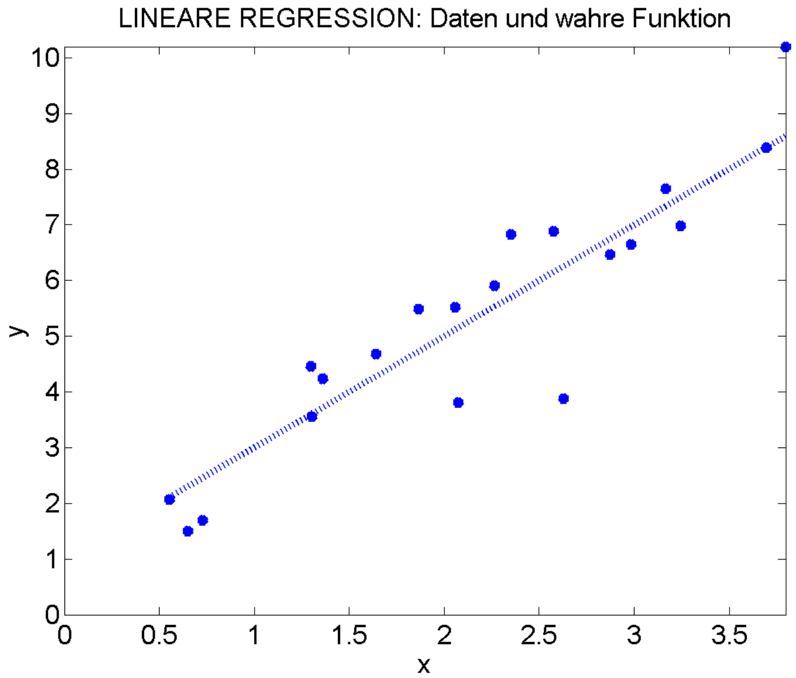
$$\mathbf{w} = (w_0, w_1)^T$$

Squared error:

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

Goal:

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



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

Least-squares Estimator in General

General Model:

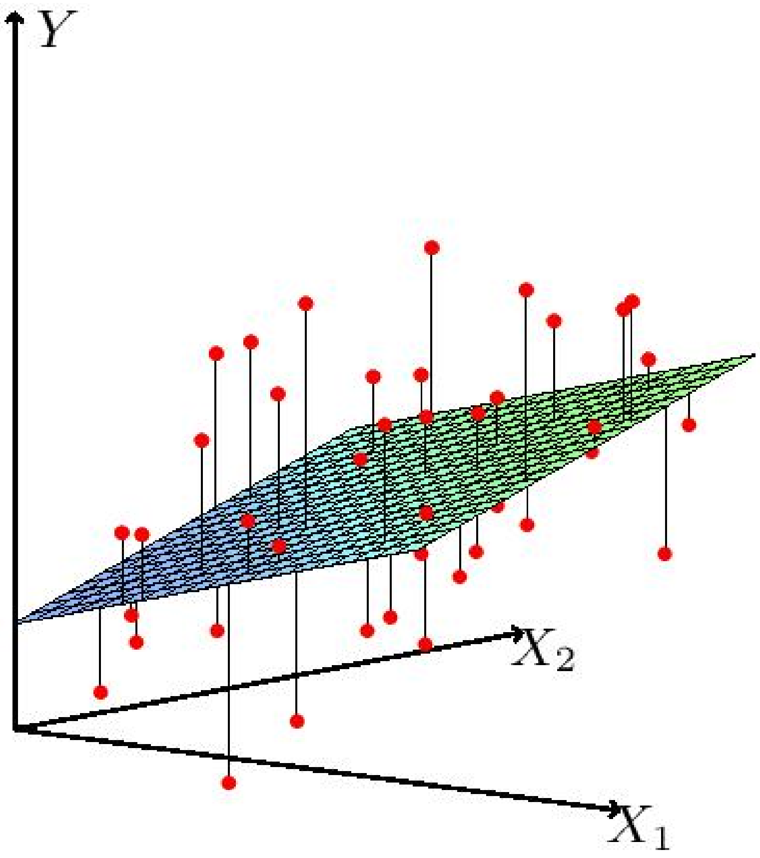
$$\widehat{y}_i = f(\mathbf{x}_i, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j x_{i,j}$$

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

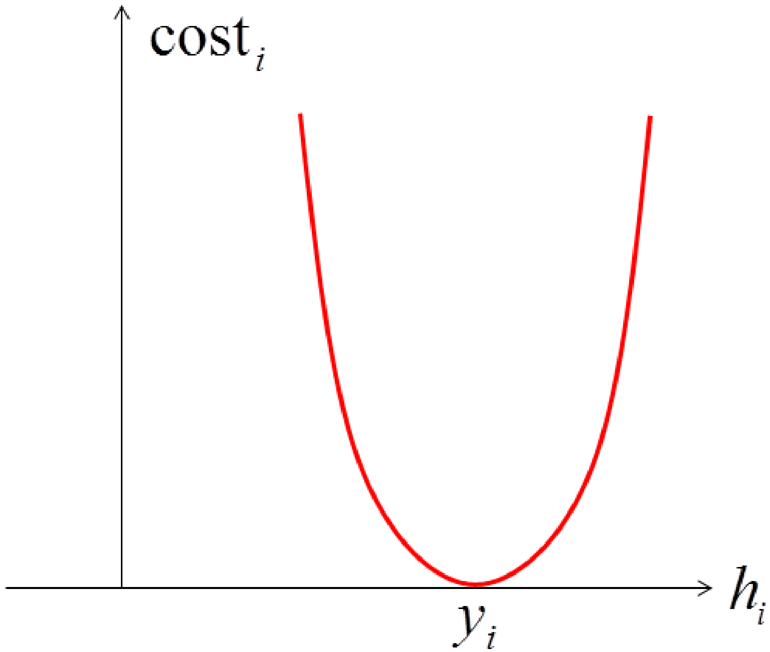
$$\mathbf{w} = (w_0, w_1, \ldots w_{M-1})^T$$

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

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)

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

- A sensible learning rule is

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

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

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

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

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

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

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

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

Setting First Derivative to Zero

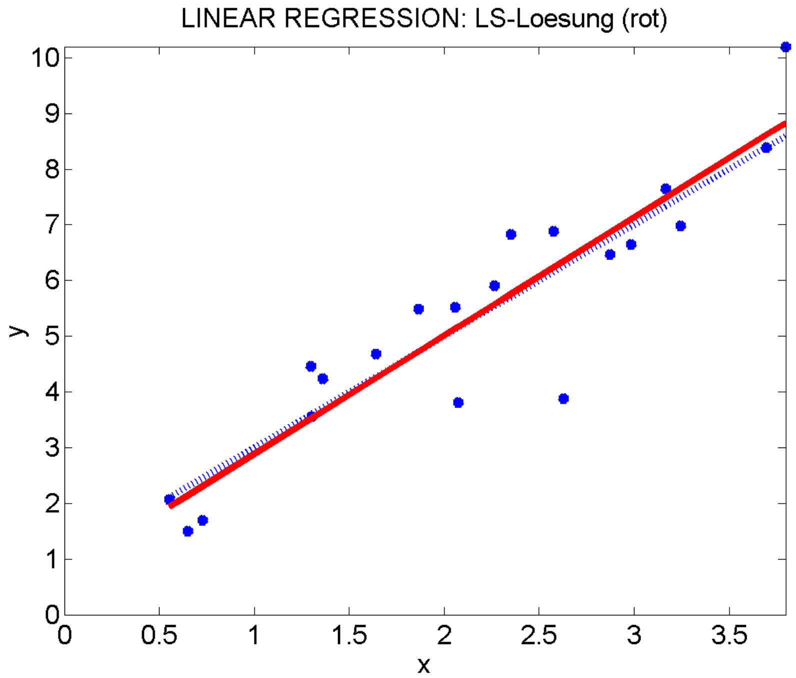
Calculating the LS-solution:

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

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

Complexity (linear in N!):

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



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

Alternative Convention

Comment: one also finds the conventions:

$$\frac{\partial}{\partial \mathbf{x}} A\mathbf{x} = A \qquad \frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T \mathbf{x} = 2\mathbf{x}^T \qquad \frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T A \mathbf{x} = \mathbf{x}^T (A + A^T)$$

Thus

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

This leads to the same solution

Stability of the Solution

- When $N >> M$, the LS solution is stable (small changes in the data lead to small changes in the parameter estimates)
- When $N < M$ then there are many solutions which all produce 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

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

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

Derivation:

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

Example: Correlated Input with no Effect on Output (Redundant Input)

- Three data points are generated as (system; true model)

$$y = 0.5 + x_1 + \epsilon_i$$

  Here, ϵ_i is independent noise

- Model 1 (correct structure)

$$f_{\mathbf{w}}(\mathbf{x}) = w_0 + w_1 x_1$$

- Training data for Model 1:

x_1	y
-0.2	0.49
0.2	0.64
1	1.39

- The LS solution gives $\mathbf{w}_{ls} = (0.58, 0.77)^T$

- In comparison, the true parameters are: $\mathbf{w} = (0.50, 1.00)^T$. The parameter estimates are reasonable, considering that only three training patterns are available

Model 2

- For Model 2, we generate a second correlated input

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

  Again, δ_i is uncorrelated noise

- Model 2 (redundant additional input)

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

Data of Model 2:

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

- The least squares solution gives $\mathbf{w}_{ls} = (0.67, -136, 137)^T$!!! The parameter estimates are far from the true parameters: This might not be surprising since $M = N = 3$

Model 2 with Regularisation

- As Model 2, only that large weights are penalized
- The penalized least squares solution gives $\mathbf{w}_{pen} = (0.58, 0.38, 0.39)^T$, also difficult to interpret !!!
- (Compare: the LS-solution for Model 1 gave $\mathbf{w}_{ls} = (0.58, 0.77))^T$

Performance on Training Data for the Models

- 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

- Thus, if we only consider the training error, we would prefer Model 2 without regularization

Performance on Test Data for the Models

- 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 (not shown)

- As a conclusion: Model 1, which corresponds to the system performs best. For Model 2 (with additional correlated input) the penalized version gives best predictive results, although the parameter values are difficult to interpret. Without regularization, the prediction error of Model 2 on test data is large. Asymptotically, with $N \to \infty$, Model 2 might learn to ignore the second input and w_0 and w_1 converge to the true parameters. **Thus, regularization helps predictive performance but does not lead to interpretable parameters, which is why it is not often used in**

classical statistical analysis. In Machine Learning, where we care mostly about predictive performance, regularization is the standard!

Experiments with Real World Data: Data from Prostate Cancer Patients

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

10-times cross validation error	LS	0.586
	Best Subset (3)	0.574
	Ridge (Penalized)	0.540

GWAS Study

Trait (here: the disease systemic sclerosis) is the output and the SNPs are the inputs. The major allele is encoded as 0 and the minor allele as 1. Thus w_j is the influence of SNP j on the trait. Shown is the (log of the p-value) of w_j ordered by the locations on the chromosomes. The weights can be calculated by penalized least squares (ridge regression)