Linear Regression

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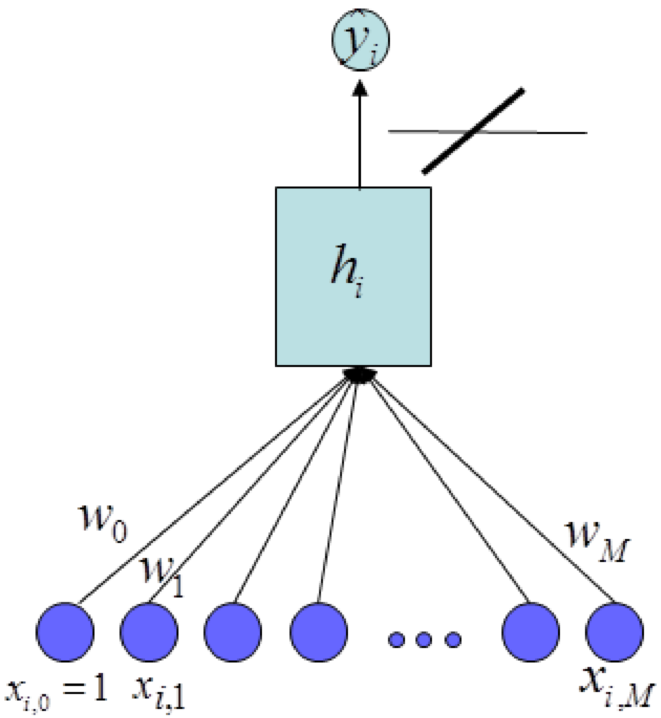
2018

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

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

(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, we take $M = 1$ (although linear regression is often applied to high-dimensional inputs)

Least-squares Estimator for Regression

One-dimensional regression:

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

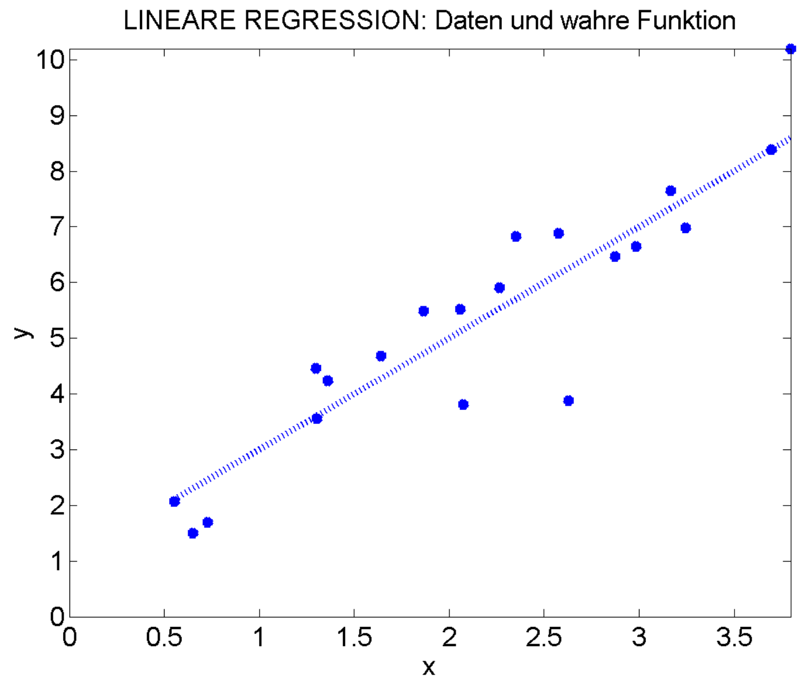
$$\mathbf{w} = (w_0, w_1)^T$$

Squared error:

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

Goal:

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



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

Least-squares Estimator in Several Dimensions

General Model:

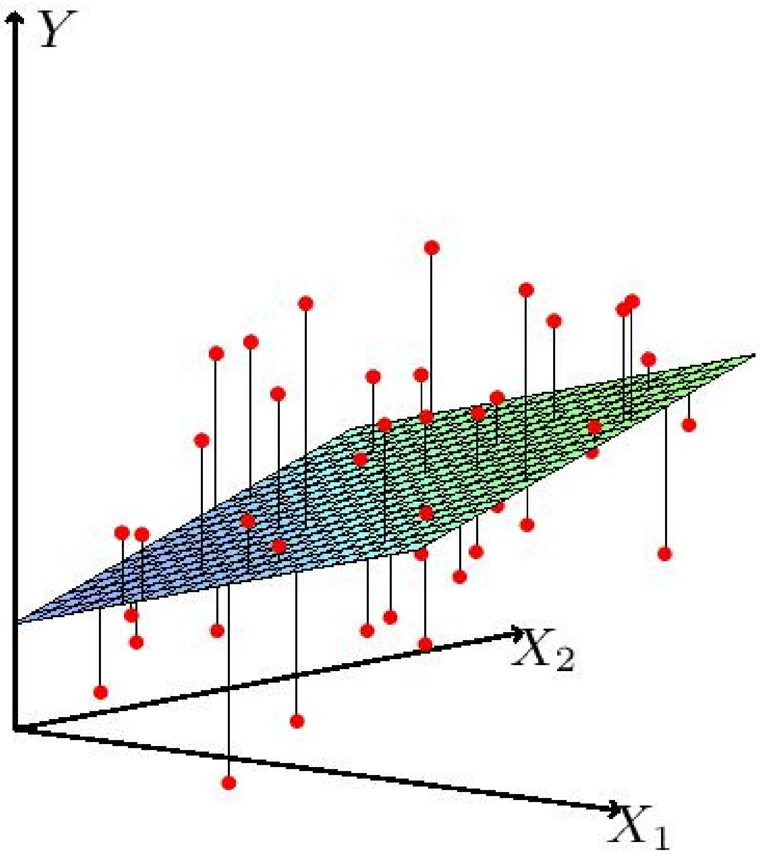
$$\widehat{y}_i = f_{\mathbf{w}}(\mathbf{x}_i) = w_0 + \sum_{j=1}^{M} w_j x_{i,j}$$

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

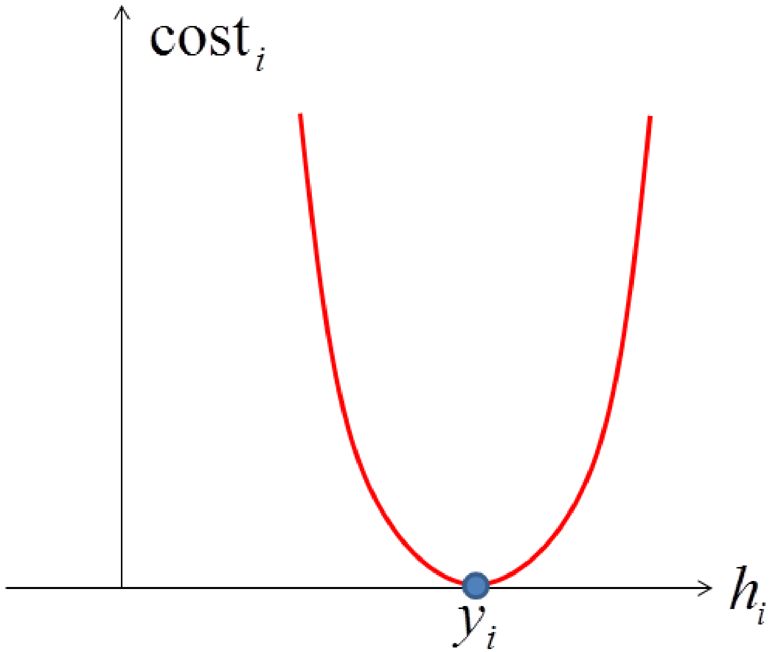
$$\mathbf{w} = (w_0, w_1, \ldots w_M)^T$$

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

Linear Regression with Several Inputs



Contribution to the Cost Function of one Data Point



Predictions as Matrix-vector product

The vector of all predictions at the training data is

$$\hat{\mathbf{y}} = \begin{pmatrix} \widehat{y}_1 \\ \widehat{y}_2 \\ \dots \\ \widehat{y}_N \end{pmatrix} = \mathbf{X}\mathbf{w}$$

Gradient Descent Learning

- Initialize parameters (typically using small random numbers)
- Adapt the parameters in the direction of the negative gradient
- With $f_{\mathbf{w}}(\mathbf{x}_i) = \sum_{j=0}^{M} w_j x_{i,j}$

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

- The parameter gradient is (Example: w_j)

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

- 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 (SGD)
- Let $\mathbf{x}_t$ and y_t be the training pattern in iteration t. The we adapt, $t = 1, 2, \ldots$

$$w_j \longleftarrow w_j + \eta(y_t - \hat{y}_t)x_{t,j} \quad j = 0, 1, 2, \ldots, M$$

- $\eta > 0$ is the learning rate, typically $0 < \eta << 0.1$
- This is identical to the Perceptron learning rule. For the Perceptron $y_t \in \{-1, 1\}$, $\hat{y}_t \in \{-1, 1\}$

Analytic Solution

- The ADALINE is optimized by SGD
- Online Adaptation: a physical system constantly produces new data: the ADALINE (SGD in general) can even track changes in the system
- With a fixed training data set the least-squares solution can be calculated analytically in one step (least-squares regression)

Cost Function in Matrix Form

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

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

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

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

Necessary Condition for an Optimum

- A necessary condition for an optimum is that

$$\left.\frac{\partial \text{cost}(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_{opt}} = 0$$

One Parameter: Explicit

- $f_w(x_1) = x_1 w_1$ and $\text{cost}(w_1) = \sum_{i=1}^{N} (y_i - x_{i,1} w_1)^2$
- (chain rule: inner derivative times outer derivative)

$$\frac{\partial \text{cost}(w_1)}{\partial w_1} = \sum_{i=1}^{N} \frac{\partial (y_i - x_{i,1} w_1)}{\partial w_1} 2(y_i - x_{i,1} w_1)$$

$$= -2 \sum_{i=1}^{N} x_{i,1}(y_i - x_{i,1} w_1) = -2 \sum_{i=1}^{N} x_{i,1} y_i + 2 w_1 \sum_{i=1}^{N} x_{i,1} x_{i,1}$$

- Thus

$$w_{1,l} = \left(\sum_{i=1}^{N} x_{i,1} x_{i,1} \right)^{-1} \sum_{i=1}^{N} x_{i,1} y_i$$

One Parameter: in Vector Notation

- $f_w(x_1) = x_1 w_1$ and $\text{cost}(w_1) = (\mathbf{y} - \bar{\mathbf{x}}_1 w_1)^T(\mathbf{y} - \bar{\mathbf{x}}_1 w_1)$, where $\bar{\mathbf{x}}_1 = (x_{1,1}, \ldots, x_{N,1})^T$

- (chain rule: inner derivative times outer derivative)

$$\frac{\partial \text{cost}(w_1)}{\partial w_1} = \frac{\partial(\mathbf{y} - \bar{\mathbf{x}}_1 w_1)}{\partial w_1} 2(\mathbf{y} - \bar{\mathbf{x}}_1 w_1)$$

$$= -2\bar{\mathbf{x}}_1^T(\mathbf{y} - \bar{\mathbf{x}}_1 w_1) = -2\bar{\mathbf{x}}_1^T \mathbf{y} + 2 w_1 \bar{\mathbf{x}}_1^T \bar{\mathbf{x}}_1$$

- Thus

$$w_{1,ls} = \left(\bar{\mathbf{x}}_1^T \bar{\mathbf{x}}_1\right)^{-1} \bar{\mathbf{x}}_1^T \mathbf{y}$$

General Case

- $f_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^T\mathbf{w}$ and $\text{cost}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$
- (chain rule: inner derivative times outer derivative)

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

$$= -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{w}\mathbf{X}^T\mathbf{X}$$

- Thus

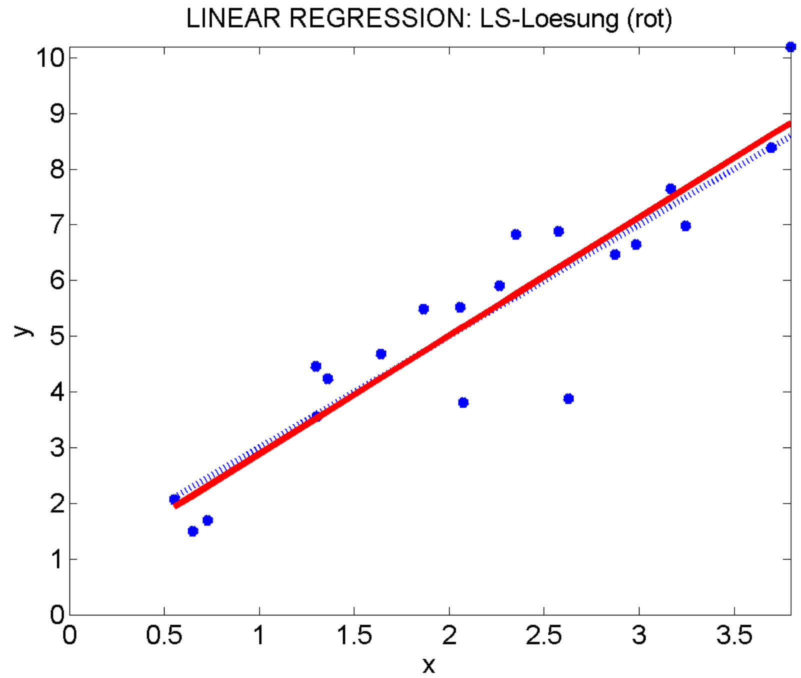
$$\mathbf{w}_{ls} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

Setting First Derivative to Zero

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

Complexity (linear in N):

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



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

Derivatives of Vector Products

- We have used

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

- Comment: one also finds the conventions,

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

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 $\sum_{i=0}^{M} w_i^2 = \mathbf{w}^T\mathbf{w}$ (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

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

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

Derivation:

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

ADALINE-Learning Rule with Weight Decay

- Let $\mathbf{x}_t$ and y_t be the training pattern in iteration t. Then we adapt, $t = 1, 2, \ldots$

$$w_j \longleftarrow w_j + \eta[(y_t - \widehat{y}_t)x_{t,j} - \frac{\lambda}{N} w_j] \quad j = 0, 1, 2, \ldots, M$$

Toy Example: Univariate Model (Pearson Correlation Coefficient)

- We generated $N = 100$ data points with $M = 3$ (no bias)
- x_1 and x_2 are highly correlated. x_3 is independent from x_1, x_2, and y
- We generate output data with $y = x_1 + \epsilon$, where ϵ stands for independent noise with standard deviation 0.2 and thus variance of 0.04. Thus ground truth parameters are $\mathbf{w}_{true} = (1, 0, 0)^T$. Note that, y causally only depends on x_1
- All variables are normalized to 0 mean and variance 1.
- In unit variate models, with only one input, the weights are identical to the sample Pearson correlation coefficients (here: $r_j = \sum_i y_i x_{i,j}/N$) between the output and the input, I get $r_1 = 0.99, r_2 = 0.96, r_3 = -0.21$
- A deeper analysis (see Appendix) reveals that the estimate r_1 has a mean of 1 and a standard deviation of 0.02. r_1 reflects the dependency of y on x_1

- The second coefficient, $r_2 = 0.96$, does not reflect a causal effect, but reflects the fact that x_1 and x_2 are highly correlated, and thus also y and x_2 (correlation does not imply causality). A deeper analysis (see Appendix) reveals that with perfect correlation between x_1 and x_2, the estimate r_1 also would have a mean of 1 and a standard deviation of 0.02

- The third value r_3 is correctly closer to 0, but not really small in magnitude. A deeper analysis (see Appendix) reveals that the estimate r_3 has a mean of 0 and a standard deviation of approximately of 0.1

Toy Example: Least Squares Regression

- We get experimentally:

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 100 & 98 & -18 \\ 98 & 100 & -16 \\ -18 & -16 & 100 \end{bmatrix}$$

Approximately $N\text{cov}(\mathbf{x})$; we see the strong correlation between x_1 and x_2

$$(\mathbf{X}^T\mathbf{X})^{-1} = \begin{bmatrix} 0.255 & -0.249 & 0.007 \\ -0.249 & 0.253 & -0.005 \\ 0.007 & -0.005 & 0.010 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{y} = (99, 97, -20)^T$$

This is approximately $N\mathbf{r}$; we see the strong correlation between both x_1 and x_2 with y

Toy Example: Least Squares Regression (cont'd)

- We get

$$\mathbf{w}_{ls} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = (1.137, -0.150, -0.018)^T$$

- Interestingly, linear regression pretty much identifies the correct causality, with $w_{ls,1} \approx 1$ and $w_{ls,2} \approx 0$!

- A deeper analysis (see Appendix) reveals that $w_{ls,1}$ has a mean of 1 and a standard deviation of 0.1. So the estimator is unbiased but the uncertainty is larger then in the unit variate analysis

- $\widehat{w}_2$ has **mean of zero** and a standard deviation of 0.1. Thus the bias is removed if compared to Pearson!

- $w_{ls,1}$ and $w_{ls,2}$ are negatively correlated. Note, that $w_{ls,1} + w_{ls,2} = 0.987$ which is close to the true 1.

- $w_{ls,3} = -0.018$ is much closer to 0 than the sample Pearson correlation coefficient $r_3 = -0.21$

- A deeper analysis (see Appendix) reveals that $w_{ls,3}$ has a mean of 0 and a standard deviation of 0.02. Here it is important to see that the standard deviation of the spurious input is largely reduced!

- Intuitive explanation: Consider that I can write the cost function as $\sum_i([y_i - w_1 x_{i,1} - w_2 x_{i,2}] - w_3 x_{i,3})$. Thus $w_3 x_{i,3}$ only needs to fit the residual target $[y_i - w_1 x_{i,1} - w_2 x_{i,2}]$ instead of the original target y_i.

- Overall, in regression, the causal influence of x_1 stands out much more clearly! Both the influence of the correlated input x_2 and the noise input x_3 are largely reduced

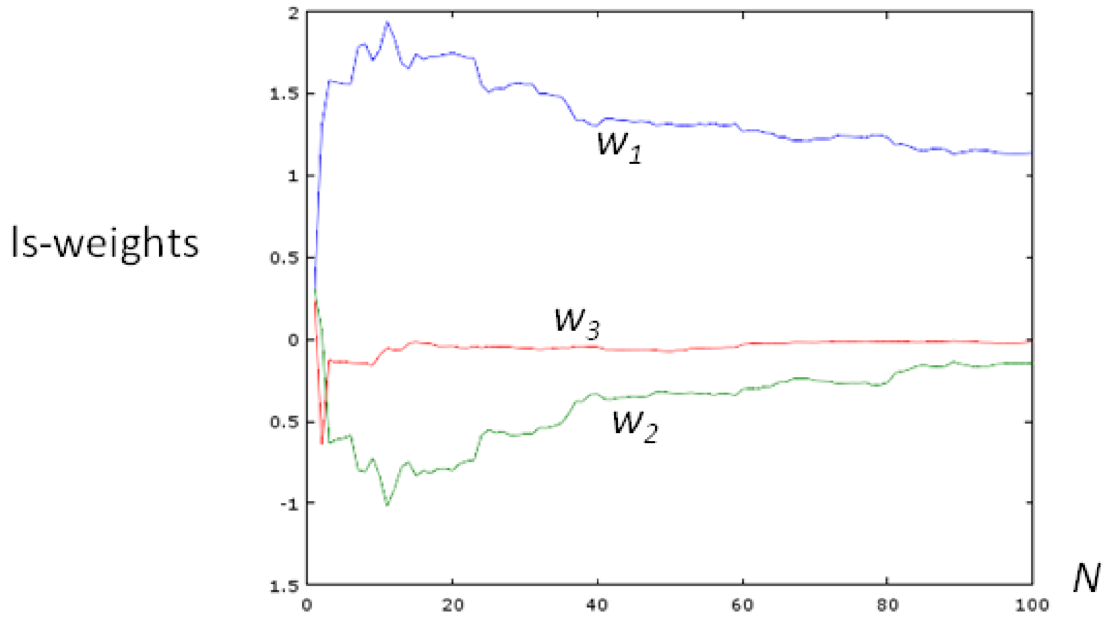
- Application in healthcare: Same data. Consider that x_2 is a medication and y the outcome. If I do a univariate analysis, I would see a strong positive influence of x_2 on y (the medication works). Only if I include the so-called confounder x_1 in the regression model, it becomes clear that the confounder x_1 is the cause and not the treatment x_2. The treatment has no significant effect!

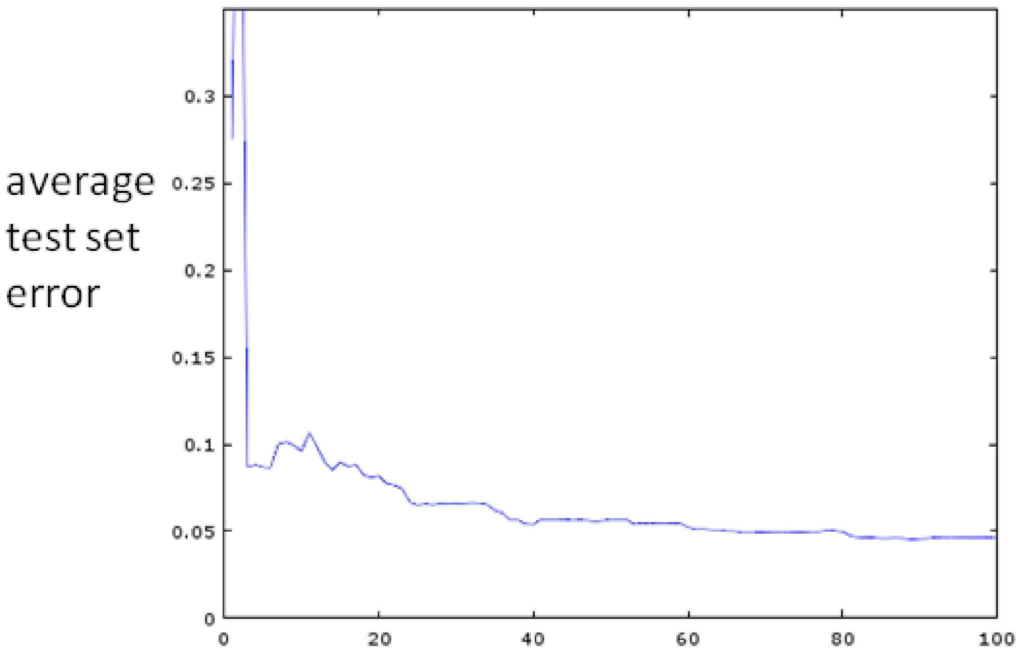
Least Squares Regression:

With small N, weights are unstable and test set error is large

With $N>50$, weights become stable

The test set error converges to the noise variance of *0.04*





Toy Example: Penalized Least Squares Regression

- We get with $\lambda = 0.6$:

$$\mathbf{X}^T\mathbf{X} + \lambda I = \begin{bmatrix} 100.6 & 98 & -19 \\ 98 & 100.6 & -17 \\ -19 & -17 & 100.6 \end{bmatrix}$$

$$(\mathbf{X}^T\mathbf{X} + \lambda I)^{-1} = \begin{bmatrix} 0.197 & -0.191 & 0.005 \\ -0.191 & 0.195 & -0.003 \\ 0.005 & -0.003 & 0.010 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{y} = (99, 97, -20)^T$$

$$\mathbf{w}_{pen} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y} = (0.990, -0.005, -0.021)^T$$

- Note that $\mathbf{w}_{pen,2}$ is even closer to ground truth!

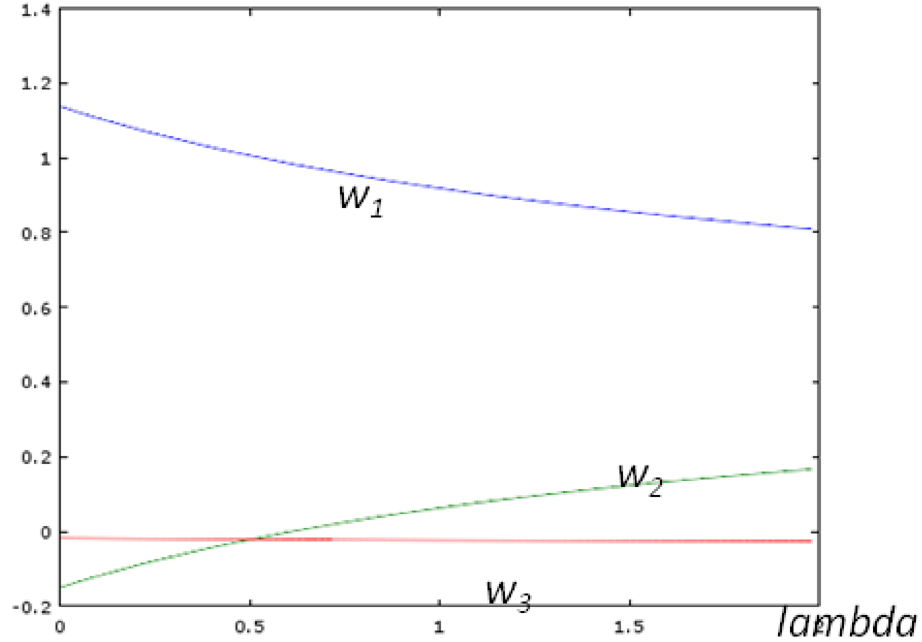
Penalized Least Squares

With large *lambda*, w_1 and w_2 converge to identical values

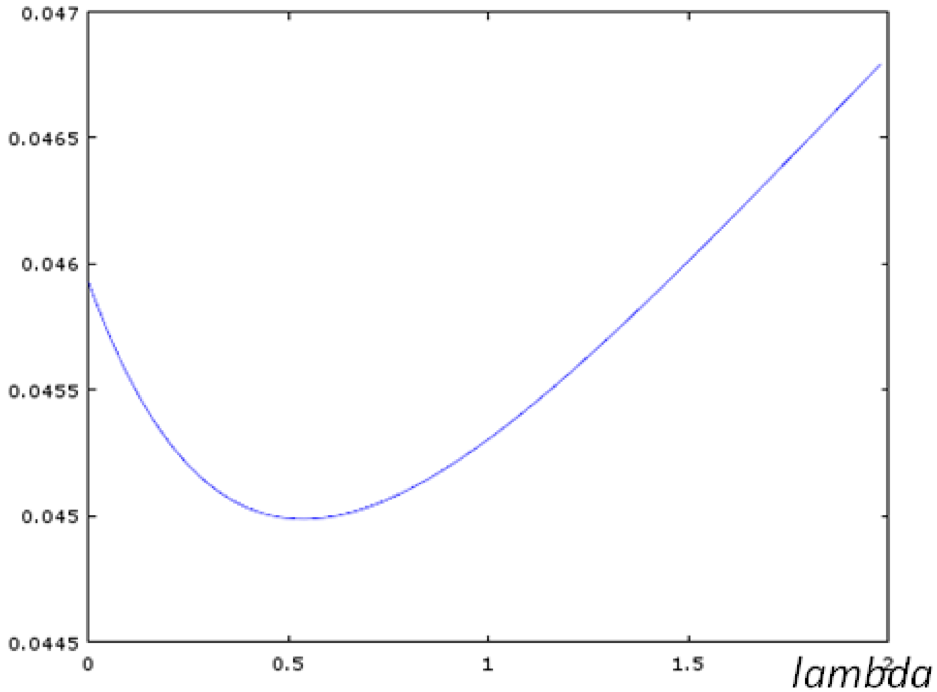
The test set error show that *lambda = 0.6* is a good value

Around *lambda = 0.6* the weight estimates are *(0.98, 0.00, -0.02)*

Penalized Least Squares -weights



average test set error

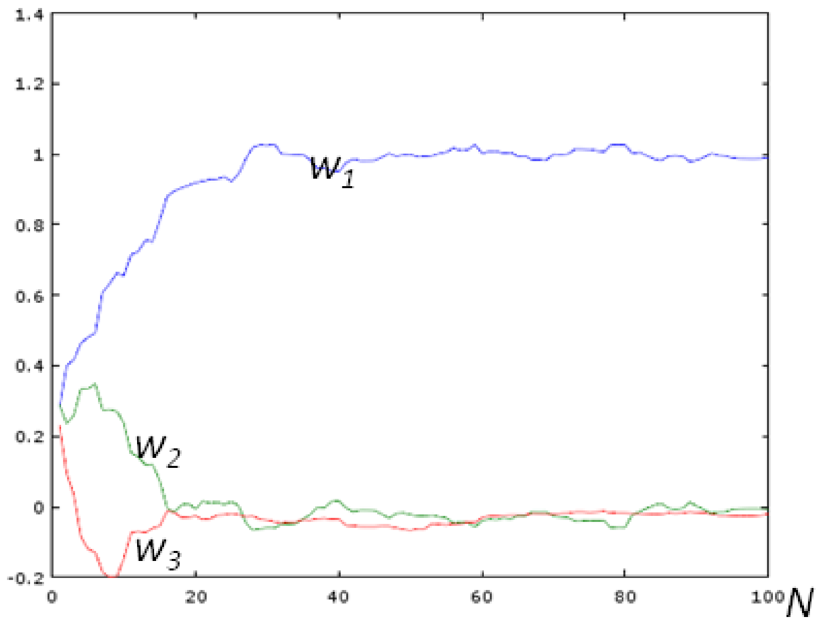


Penalized Least Squares Regression *(lambda = 0.6)*:

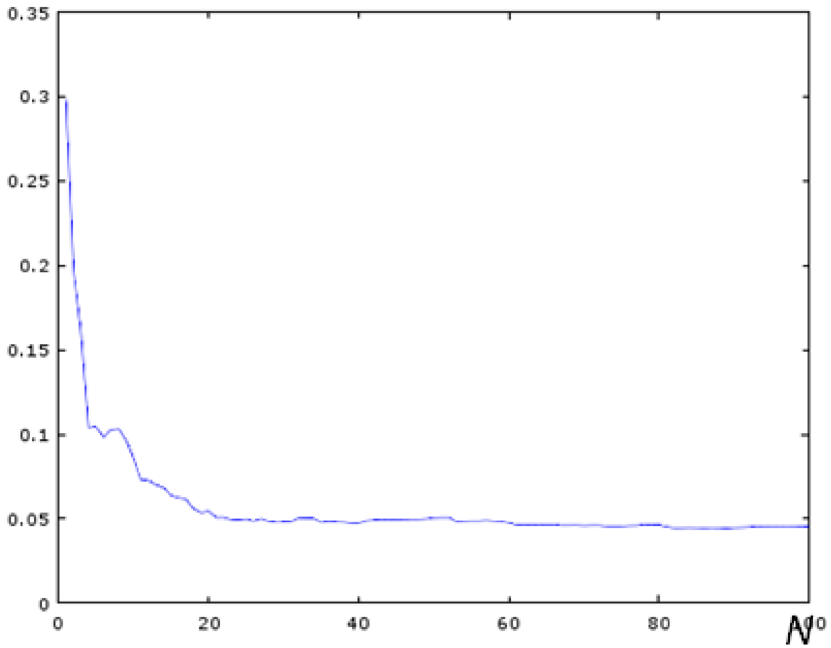
With small *N*, weights are close to *0* and test set error is large

With *N>50*, weight estimates and test set error and test set error converges to the noise variance of *0.04*

Penalized Least Squares -weights



average test set error



Remarks

- The Pearson correlation coefficient does not reflect causality
- The regression coefficients display causal behavior, much more closely
- If one is only interested in prediction accuracy: adding inputs liberally in regression can be beneficial if regularization is used (in ad placements and ad bidding, hundreds or thousands of features are used)
- The weight parameters of useless (noisy) features become close to zero with regularization (ill-conditioned parameters)
- Regularization is especially important when $N \approx M$, and $N < M$
- If parameter interpretation is essential or if, for computational reasons, one wants to keep the number of inputs small:
- — Forward selection; start with the empty model; at each step add the input that reduces the error most

- — Backward selection (pruning); start with the full model; at each step remove the input that increases the error the least
- But no guarantee, that one finds the best subset of inputs or that one finds the true inputs

Experiments with Real World Data: Data from Prostate Cancer Patients

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

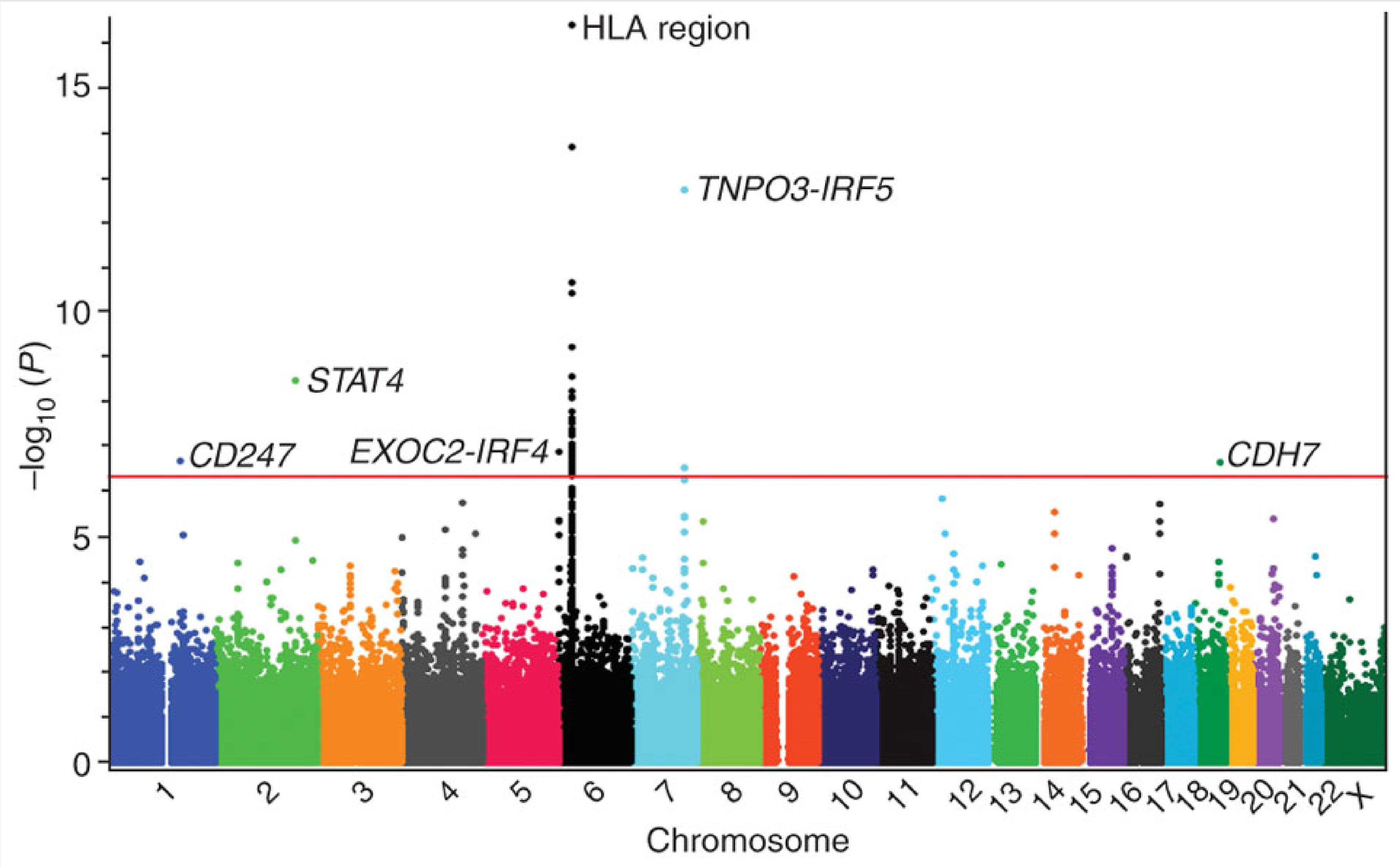
	LS	0.586
10-times cross validation error	Best Subset (3)	0.574
	Ridge (Penalized)	0.540

Examples where High-dimensional Linear Systems are Used

- Ranking in search engines (relevance of a web page to a query)
- Ad placements: where to put which ad for a user
- GWAS

Genome-wide Association Study (GWAS)

- 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)
- Solely based on the Pearson correlation, the plot would show many more (non-causal) associations. The regression analysis reduces the apparent influence of noncausal correlated inputs and the influence of uncorrelated inputs
- In practice one often uses an elastic net penalty: $\lambda_2 \sum_j w_j^2 + \lambda_1 \sum_j |w_j|$ where the lasso penalty $\lambda_1 \sum_j |w_j|$ increases sparsity



HLA region
TNPO3-IRF5
STAT4
CD247
EXOC2-IRF4
CDH7
−log10 (P)
15
10
5
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
X
Chromosome

Appendix: A Deeper Analysis of Pearson versus Regression*

- The Pearson correlation coefficient is in the mean approximately $(1, 1, 0)$. The variance of r_1, and r_2 can be estimated as $\text{var} = \sigma^2/N = 0.04/100 = 0.0004$ and standard deviation $\text{stdev} = \sqrt{\text{var}} = 0.02$. For r_3 we get a variance $\text{var}(r_3) = \text{var}(y)/N = 1/N = 0.01$, and a standard deviation of $\text{stdev}(r_3) = 0.1$. Comment: r_2 does not reflect the true dependency; the variance of r_3 is relatively large.

- Since linear regression is unbiased, the parameter estimates have mean $1, 0, 0$ (unbiased solutions). We get for the covariances

$$\text{cov}(\mathbf{w}_{ls}) = \sigma^2 (X^T X)^{-1}$$

The variances are then (we consider the diagonal terms)

$$\text{var}(w_{ls,1}) = \text{var}(w_{ls,2}) \approx 0.04 \times 0.25 = 0.01$$

$$\text{var}(w_{ls,3}) \approx 0.04 \times 0.01 = 0.0004,$$

and

$$\text{stdev}(w_{ls,1}) = \text{stdev}(w_{ls,2}) \approx 0.2$$

$$\text{stdev}(w_{ls,3}) \approx 0.02$$

- Thus the estimates are unbiased; the uncertainty of $w_{ls,3}$ is greatly reduced and thus closer to zero!