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

$$h(\mathbf{x}) = \sum_{j=0}^{M} w_j x_j$$

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

• The activation is the output (no thresholding)

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

• Regression: the target function can take on real values

Effect of a Single Binary Input

- Consider only binary inputs with $x_{i,j} \in \{0, 1\}$
- When x_{i,j} switches from 0 to 1 and the other inputs remain fixed (intervention), the j-th input adds to the output the quantity w_j, independent of context, i.e., independent of the other inputs! (the average causal effect is identical to the individual causal effect)
- Recall that for the perceptron, the effect of an input on the output does critically depend on context: When $x_{i,j}$ switches from 0 to 1 and the other inputs remain fixed (intervention), dependent on the other inputs, the output might stay as is, or changes from 1 to -1 or from -1 to 1

Method of Least Squares

• Squared-loss cost function:

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

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

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

• 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:

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

Goal:

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



Least-squares Estimator in Several Dimensions

General Model:

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

$$\mathbf{w} = (w_0, w_1, \dots, w_M)^T$$
$$\mathbf{x}_i = (1, x_{i,1}, \dots, x_{i,M})^T$$

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

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

Gradient Descent Learning

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

• With
$$f_{\mathbf{w}}(\mathbf{x}_i) = \sum_{j=0}^{M} w_j x_{i,j}$$

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

• The parameter gradient is (Example:
$$w_j$$
)

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

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

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

- $\eta > 0$ is the learning rate, typically $0 < \eta << 0.1$
- Depending again on the difference ("delta") $(y_t \widehat{y}_t)$, this is again called a delta rule
- This is identical to the Perceptron learning rule (see Appendix in the lecture on the Perceptron). But, for the Perceptron $y_t \in \{-1, 1\}$, and $\hat{y}_t \in \{-1, 1\}$

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

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

$$= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$
$$\mathbf{y} = (y_1, \dots, y_N)^T$$

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

Necessary Condition for an Optimum

• A necessary condition for an optimum is that

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

One Parameter: Explicit

•
$$f_w(x_1) = x_1 w_1$$
 and $\operatorname{cost}(w_1) = \sum_{i=1}^N (y_i - x_{i,1} w_1)^2$

• (chain rule: inner derivative times outer derivative)

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

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

• Thus

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

General Case

•
$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$$
 and $COSt(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$

• (chain rule: inner derivative times outer derivative)

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

• Thus

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

Setting First Derivative to Zero



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

LS-Regression (octave/matlab)

```
octave:190> % LS-REGRESSION
octave:190> N = 6;
octave:191> M=4:
octave:192> noiseStdv = 0.2;
octave:193> X = randn(N, M); % design matrix
octave:194> wtrue = rand(M, 1); % true paraeters
octave:195> wtrue'
ans =
   0.79811 0.39086 0.95365 0.67450
octave:196> % target vector; noise variance = 0.2^2
octave:196> y = X * wtrue + noiseStdv *randn(N,1);
octave:197> % least squares weights
octave:197> wls = inv(X'*X) * X' * v;
octave:198> wls'
ans =
   0.85725 0.21407 1.04269 0.79409
octave:199>
octave:199> % average training cost:
octave:199> XTest = randn(N, M); % design matrix
octave:200> ytest = XTest * wtrue + noiseStdv *randn(N,1);
octave:201> AverageCostTrain = (v - X*wls)' * (v - X*wls)/N
AverageCostTrain = 0.0039304
octave:202> AverageCostTest = (ytest - XTest*wls)' * (ytest - XTest*wls)/N
AverageCostTest = 0.047907
```

Derivatives of Vector Products

• We have used

$$\frac{\partial}{\partial \mathbf{w}} \mathbf{X} \mathbf{w} = \mathbf{X}^T \quad \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T \mathbf{w} = 2\mathbf{w} \quad \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T \mathbf{X} \mathbf{w} = (\mathbf{X} + \mathbf{X}^T) \mathbf{w}$$

• Comment: one also finds the conventions,

$$\frac{\partial}{\partial \mathbf{w}} \mathbf{X} \mathbf{w} = \mathbf{X} \quad \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T \mathbf{w} = 2\mathbf{w}^T \quad \frac{\partial}{\partial \mathbf{w}} \mathbf{w}^T \mathbf{X} \mathbf{w} = \mathbf{w}^T (\mathbf{X} + \mathbf{X}^T)$$

Machine Learning as an Inverse Problem

- $\bullet \ \mbox{The map } \mathbf{w} \mapsto \mathbf{y} = \mathbf{X} \mathbf{w}$ is the forward model
- The map $\mathbf{y} \mapsto \mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ is the inverse model
- X⁺ = (X^TX)⁻¹X^T is called the Moore-Penrose pseudo inverse (generalized inverse); (Roger Penrose won the 2020 Nobel Prize in Physics)
- Machine learning is an "inverse" problem

Stability of the Solution

- When $N >> M_p$, the LS solution is stable (small changes in the data lead to small changes in the parameter estimates)
- When $N < M_p$ then there are many solutions which all produce zero training error
- Of all these solutions, one selects the one that minimizes $\sum_{j=0}^{M} w_j^2 = \mathbf{w}^T \mathbf{w}$ (regularised solution)
- \bullet Even with $N>M_p$ 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

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

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

Derivation:

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

```
octave:190> % LS-REGRESSION
                          octave:190> N = 6;
PLS-Regression
                          octave:191> M=4;
                          octave:192> noiseStdv = 0.2;
(octave/matlab)
                          octave:193> X = randn(N, M); % design matrix
                          octave:194> wtrue = rand(M, 1); % true paraeters
                          octave:195> wtrue'
                          ans =
                             0.79811 0.39086 0.95365 0.67450
                          octave:196> % target vector; noise variance = 0.2^2
                          octave:196> y = X * wtrue + noiseStdv *randn(N,1);
                          octave:197> % least squares weights
                          octave:197> wls = inv(X'*X) * X' * y;
                          octave:198> wls'
                          ans =
                             0.85725 0.21407 1.04269 0.79409
                          octave:199>
                          octave:199> % average training cost:
                          octave:199> XTest = randn(N, M); % design matrix
                          octave:200> ytest = XTest * wtrue + noiseStdv *randn(N,1);
                          octave:201> AverageCostTrain = (y - X*wls)' * (y - X*wls)/N
                          AverageCostTrain = 0.0039304
                          octave:202> AverageCostTest = (ytest - XTest*wls)' * (ytest - XTest*wls)/N
                          AverageCostTest = 0.047907
                          octave:203>
                          octave:203> % PLS-REGRESSION
                          octave:203> lam=0.2
                          lam = 0.20000
                          octave:204> wpls = inv(X'*X + lam* eye(M)) * X' * y;
                          octave:205> wpls'
                          ans =
                             0.80884 0.25011 0.97113 0.70296
                          octave:206> AverageCostTrain = (y - X*wpls)' * (y - X*wpls)/N
                          AverageCostTrain = 0.0093865
                          octave: 207> AverageCostTest = (vtest - XTest*wpls)' * (vtest - XTest*wpls)/N
                          AverageCostTest = 0.027686
```

ADALINE-Learning Rule with Weight Decay

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

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

Toy Example

- We generated N = 100 data points with M = 3 inputs ($w_0 = 0$ is known)
- x_1 and x_2 are highly correlated (x_2 is generated from x_1)
- x_3 is independent of all the other variables: 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 the true parameters are $\mathbf{w}_{true} = (1, 0, 0)^T$; Note that, y causally only depends on x_1
- Thus the **true function** is

$$y = 1 \times x_1 + 0 \times x_2 + 0 \times x_3 + \epsilon$$

- Thus, $\mathbf{w}_{true} = (1, 0, 0)^T$ (without w_0)
- All variables x_1, x_2, x_3, y are normalized to zero mean and variance 1





(penalized least squares)

Toy Example: One-dimensional Model

• In one-dimensional models, with only one input, the weights are identical to the sample **Pearson correlation coefficients** (here: $\hat{w}_j = \hat{r}_j = \sum_i y_i x_{i,j}/N$) between the output and the input (equality only because of the normalization of the variables) $-1 \leq \hat{r}_j \leq 1$

• I obtain
$$\hat{r}_1 = \hat{w}_1 = 0.99$$
, $\hat{r}_2 = \hat{w}_2 = 0.96$, $\hat{r}_3 = \hat{w}_3 = -0.21$

• Explicitly, the three **one-dimensional models** are

$$\hat{y} = 0.99x_1$$
 $\hat{y} = 0.96x_2$ $\hat{y} = -0.21x_3$

In general, the expected Pearson correlation coefficient is defined as

$$r_{x,y} = cov_{xy}/(stdev_x stdev_y)$$

Toy Example: One-dimensional Model (cont'd)

- The first Pearson correlation, $\hat{r}_1 = 0.99$, reflects the causal effect; its expected value is 1, in the example
- The second Pearson correlation, $\hat{r}_2 = 0.96$, 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). Its expected value is 1, in the example
- The third Pearson correlation, $\hat{r}_3 = -0.21$ is correctly closer to 0, but not really small in magnitude (its expected value is 0, in the example).

Toy Example: Least Squares Regression

• We get:

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

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

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

Finally,

$$X^T y = (99, 97, -20)^T$$

This is $N \times (\hat{r}_1, \hat{r}_2, \hat{r}_3)^T$! We see the strong correlation between both x_1 and x_2 with y

Toy Example: Least Squares Regression (cont'd)

• We get

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

• Interestingly, linear regression pretty much identifies the correct causality, with $\hat{w}_1 \approx 1$ and $\hat{w}_2 \approx 0$! The expected value of \hat{w}_1 actually is 1 and of \hat{w}_2 actually is 0. Note the dramatic shift to 0!

Toy Example: Least Squares Regression (cont'd)

- $\hat{w}_3 = -0.018$ is much closer to 0, compared to the sample Pearson correlation coefficient ($\hat{r}_3 = -0.21$)
- Overall, in regression, the causal influence of x_1 stands out much more clearly!
- Both the influence of the correlated (non-causal) input x₂ and the noise input x₃ are largely reduced

The Power of Supervised Learning

- In regression: an input only has to model, what the other inputs could not model
- In a one-dimensional analysis: each input on its own tries to model the dependency to y as well as possible!

Toy Example: Penalized Least Squares Regression

• We get with $\lambda = 0.6$:

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

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

$$X^T y = (99, 97, -20)^T$$

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

• Note that $\hat{\mathbf{w}}_2$ is even closer to ground truth!







Application to Healthcare

- Assume same data
- Consider that x₂ is a treatment (medication) and y the outcome (healthy=1, after treatment).
- If I do a one-dimensional analysis, I would see a strong positive influence of x_2 on y
- I might conclude that the treatment 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
- I conclude that the treatment has no significant effect!
- Recipe: Do a multidimensional regression model and include all relevant inputs!

Application to Healthcare (cont'd)

- Example: Only patients without any other disease (x₁ = 1) get the treatment, but they get healthy (y = 1), independent of treatment (x₂) (since their bodies can focus on the disease of interest); still, this results in a correlation between treatment (x₂) and outcome (y)
- Fisher's hypothesis (epidemiology): A certain gene variant (x₁ = 1) causes lung cancer, but also makes you want to smoke (x₂ = 1), but smoking itself has no effect on lung cancer y; still, this results in a correlation between smoking (x₂) and outcome (y)
- Now that we can measure genetic variance: Fisher's hypothesis is (mostly) wrong
- But: Maybe a developing lung cancer makes you feel like you want to smoke





(penalized least squares)



- lung cancer
- smoking!

• Common cause (Fisher): a genetic factor makes you want to smoke and increases your chance of getting lung cancer

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 Smoking does not make a difference

- G
 - A developing lung cancer makes you want to smoke (which might relieve some strange feeling about your lung)

_C

 Smoking does not make a difference

- In all three case you see a correlation (dependency) between lung cancer and smoking
- You can predict (probabilistically) lung cancer (output) from smoking (input)

Remarks: Correlation versus Regression

- The Pearson correlation coefficients is independent of context, objective. Karl Pearson: "I interpreted that sentence of Francis Galton (1822-1911) [his advisor] to mean that there was a category broader than causation, namely correlation, of which causation was only the limit, and that this new conception of correlation brought psychology, anthropology, medicine, and sociology in large parts into the field of mathematical treatment."
- But the Pearson correlation coefficient does not reflect causality (dependencies)
- The regression coefficients display causal behavior, much more closely: *causality anal-ysis based on observed data requires complete models*
- "Gold standard": prospective randomized controlled trial (RCT): assign patients randomly to the treatment group
- In epidemiological studies RCTs are often not ethical: you cannot just tell people to start smoking; here one often needs to rely on (carefully analysed) retrospective observational studies

Remarks: Regularization

- 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 $N \approx M_p$, or when $N < M_p$
- 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

LS0.58610-times cross validation errorBest Subset (3)0.574Ridge (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 advertizement on a web page, for a user with a given user profile