Machine Learning Course - CS-433

Least Squares

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Motivation

In rare cases, one can compute the optimum of the cost function analytically. Linear regression using a mean-squared error cost function is one such case. Here the solution can be obtained explicitly, by solving a linear system of equations. These equations are sometimes called the normal equations. This method is one of the most popular methods for data fitting. It is called least squares.

To derive the normal equations, we first show that the problem is convex. We then use the optimality conditions for convex functions (see the previous lecture notes on optimization). I.e., at the optimium parameter, call it $\mathbf{w}^\star$, it must be true that the gradient of the cost function is 0. In other words, we must have that

$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}.$$

This is a system of D equations.

Normal Equations

Recall that the cost function for linear regression with a mean-square error criterion is given by

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}),$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix}.$$

We claim that this cost function is convex in the $\mathbf{w}$. There are several ways of proving this.

1. We can compute the second derivative (the Hessian) and to show that it is positive semidefinite (all its eigenvalues are non-negative). For the present case a computation shows that the Hessian has the form

   $$\frac{1}{N}\mathbf{X}^\top\mathbf{X}.$$

   This matrix is indeed positive semidefinite since it's non-zero eigenvalues are the squares of the non-zero eigenvalues of the matrix $\mathbf{X}$.

2. We can go back directly to the definitions and show that for any $\lambda \in [0,1]$ and and $\mathbf{w}_1$ and $\mathbf{w}_2$,

   $$\mathcal{L}(\lambda\mathbf{w}_1 + (1-\lambda)\mathbf{w}_2) - (\lambda\mathcal{L}(\mathbf{w}_1) + (1-\lambda)\mathcal{L}(\mathbf{w}_2)) \leq 0.$$

   A computation shows that the left-hand side can be written as

   $$-\frac{1}{2N}\lambda(1-\lambda)\|\mathbf{X}(\mathbf{w}_1 - \mathbf{w}_2)\|_2^2,$$

   which indeed is non-positive.

3. The simplest way is to observe that this function is naturally represented as the sum (with positive coefficients) of the simple terms $(y_n - \mathbf{x}_n^\top \mathbf{w})^2$. Further, each of these simple terms is the composition of a linear function with a convex function (the square function). Therefore, each of these simple terms is convex and hence the sum is convex.

Now where we know that the function is convex, let us find its minimum. If we take the gradient of this expression with respect to the weight vector $\mathbf{w}$ we get

$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N}\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}).$$

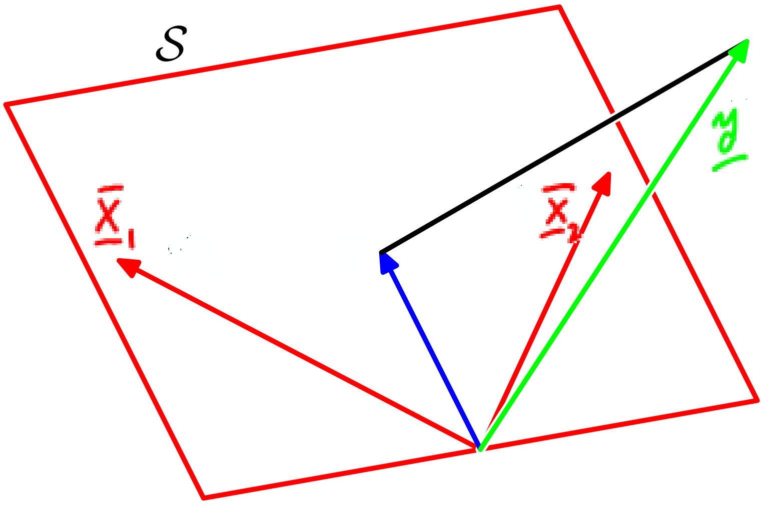
If we set this expression to 0 we get the normal equations for linear regression,

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}. \tag{1}$$

Geometric Interpretation

Let $\mathcal{S}$ denote the space spanned by the columns of $\mathbf{X}$. Note that $\mathbf{x} = \mathbf{X}\mathbf{w}$ is an element of $\mathcal{S}$. I.e., by choosing $\mathbf{w}$ we choose $\mathbf{x} \in \mathcal{S}$. What element of $\mathcal{S}$ shall we take? The normal equations tell us that the optimum choice for $\mathbf{x}$, call it $\mathbf{x}^\star$, is that element so that $\mathbf{y} - \mathbf{x}^\star$ is orthogonal to $\mathcal{S}$. In other words, we we should pick $\mathbf{x}^\star$ to be equal to the projection of $\mathbf{y}$ onto $\mathcal{S}$.

The following figure (taken from Bishop's book) illustrates



this point:

Rewriting the normal equations (1) by expanding the terms and we get

$$\mathbf{X}^\top \mathbf{X} \mathbf{w}^\star = \mathbf{X}^\top \mathbf{y}. \tag{2}$$

Least Squares

The matrix $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{D \times D}$ is called the Gram matrix. If it is invertible, we can multiply (2) by the inverse of the Gram matrix from the left to get a closed-form expression for the minimum.

$$\mathbf{w}^\star = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

We can use this model to predict a new value for an unseen datapoint (test point) $\mathbf{x}_m$:

$$\hat{y}_m := \mathbf{x}_m^\top \mathbf{w}^\star = \mathbf{x}_m^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Invertibility and Uniqueness

Note that the Gram matrix $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{D \times D}$ is invertible if and only if $\mathbf{X}$ has full column rank, or in other words $rank(\mathbf{X}) = D$.

Proof: To see this assume first that $rank(\mathbf{X}) < D$. Then there exists a non-zero vector $\mathbf{u}$ so that $\mathbf{X}\mathbf{u} = 0$. It follows that $\mathbf{X}^\top\mathbf{X}\mathbf{u} = 0$, and so $rank(\mathbf{X}^\top\mathbf{X}) < D$. Therefore, $\mathbf{X}^\top\mathbf{X}$ is not invertible.

Conversely, assume that $\mathbf{X}^\top\mathbf{X}$ is not invertible. Hence, there exists a non-zero vector $\mathbf{v}$ so that $\mathbf{X}^\top\mathbf{X}\mathbf{v} = 0$. It follows that

$$0 = \mathbf{v}^\top\mathbf{X}^\top\mathbf{X}\mathbf{v} = (\mathbf{X}\mathbf{v})^\top(\mathbf{X}\mathbf{v}) = \|\mathbf{X}\mathbf{v}\|^2.$$

This implies that $\mathbf{X}\mathbf{v} = 0$, i.e., $rank(\mathbf{X}) < D$.

Rank Deficiency and Ill-Conditioning

Unfortunately, in practice, $\mathbf{X}$ is often rank deficient.

- If $D > N$, we always have $rank(\mathbf{X}) < D$ (since row rank = col. rank)
- If $D \leq N$, but some of the columns $\mathbf{x}_{:d}$ are (nearly) collinear, then the matrix is ill-conditioned, leading to numerical issues when solving the linear system.

What this means operationally is there are now many ways of picking $\mathbf{w}$ to represent the unique projection of $\mathbf{w}$ onto $\mathcal{S}$. In fact, there is a whole subspace of solutions. We just want to find one.

So what do we do when we either have a truly rank deficient matrix $\mathbf{X}$ or $\mathbf{X}$ is badly conditioned? We use the singular-value decomposition (SVD). We will learn much more about the SVD in later lectures. We will therefore be rather brief at the moment.

Just for completeness let us write down the solution here. Let

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$$

be the SVD of $\mathbf{X}$. Here, $\mathbf{U}$ is an $N \times N$ unitary matrix.[1] The matrix $\mathbf{S}$ is of dimension $N \times D$. It has zero entries except along the diagonal where the entries are non-negative and ordered from largest to smallest. Note further that the number of non-zero entries is equal to the rank of $\mathbf{X}$. Finally, $\mathbf{V}$ is a $D \times D$ unitary matrix.
So we have

$$\begin{aligned} \mathbf{U}\mathbf{U}^\top &= \mathbf{U}^\top\mathbf{U} = \mathbf{I}_{D\times D}, \\ \mathbf{V}\mathbf{V}^\top &= \mathbf{V}^\top\mathbf{V} = \mathbf{I}_{N\times N}. \end{aligned}$$

Recall that the condition $\mathbf{U}\mathbf{U}^\top = \mathbf{I}_{D\times D}$ means that the matrix $\mathbf{U}$ has *orthonormal* (i.e., orthogonal and square norm 1) rows and that $\mathbf{U}^\top = \mathbf{U}^{-1}$. But if $\mathbf{U}\mathbf{U}^\top = \mathbf{I}_{D\times D}$ then also $\mathbf{U}^\top\mathbf{U} = \mathbf{U}^{-1}\mathbf{U} = \mathbf{I}_{D\times D}$, so that also the columns of $\mathbf{U}$ are orthonormal. Therefore, requiring that a matrix is *unitary*, is the same as requiring that it has orthonormal rows, or requiring that it has orthonormal columns.
The equation we have to solve is then of the form

$$\mathbf{V}\mathbf{S}^\top\mathbf{S}\mathbf{V}^\top\mathbf{w}^\star = \mathbf{V}\mathbf{S}^\top\mathbf{U}^\top\mathbf{y}.$$

[1] Our notation assumes that the matrix is real-valued. In this case all the matrices in the SVD are also real-valued and $\mathbf{U}$ and $\mathbf{V}$ are said to be orthogonal matrices. In the more general case of complex-valued matrices one says that the matrix is unitary. In this case the transpose operator is supposed to be intepretated as the usual transpose and complex conjugation. We will refer to $\mathbf{U}$ and $\mathbf{V}$ as unitary even though we assume that they are real-valued.

Multiplying by the left with $\mathbf{V}^\top$ we get

$$\mathbf{S}^\top \mathbf{S} \mathbf{V}^\top \mathbf{w}^\star = \mathbf{S}^\top \mathbf{U}^\top \mathbf{y}.$$

Note that this equation has in general a whole space of solutions. To find one particular one, define the so-called *pseudo-inverse* $\tilde{\mathbf{S}}$ which is a $D \times N$ matrix. On the diagonal of $\tilde{\mathbf{S}}$ take the non-zero diagonal entries of $\mathbf{S}$ and invert them. All other entries are zero. It is called a *pseudo-inverse* since $\tilde{\mathbf{S}}\mathbf{S}$ is a $D \times D$ matrix with zero entries except along the diagonal where the first $rank(\mathbf{X})$ entries are 1 and the rest are 0. And in a similar manner, $\mathbf{S}\tilde{\mathbf{S}}$ is a $N \times N$ matrix with zero entries except along the diagonal where the first $rank(\mathbf{X})$ entries are 1 and the rest are 0.
Multiply our equation from the left by $\mathbf{V}\tilde{\mathbf{S}}\tilde{\mathbf{S}}^\top$. We then have the solution

$$\mathbf{w}^\star = \mathbf{V}\tilde{\mathbf{S}}\mathbf{U}^\top \mathbf{y}.$$

Note that $\mathbf{V}\tilde{\mathbf{S}}\mathbf{U}^\top$ is known as the *pseudo-inverse* of $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$ for the same reason that $\tilde{\mathbf{S}}$ is the pseudo-inverse of $\mathbf{S}$.

Summary of Linear Regression

We have studied three types of methods:

1. Grid Search
2. Iterative Optimization Algorithms
   (Stochastic) Gradient Descent
3. Least squares
   closed-form solution, for linear MSE

Additional Notes

Closed-form solution for MAE

Can you derive closed-form solution for 1-parameter model when using MAE cost function?
See this short article: http://www.johnmyleswhite.com/notebook/2013/03/22/modes-medians-and-means-an-unifying-perspective/.

Implementation

There are many ways to solve a linear system, but using the QR decomposition is one of the most robust ways. Matlab's backslash operator and also NumPy's linalg package implement this in just one line:

```
    w = np.linalg.solve(X, y)
```

For a robust implementation, see Sec. 7.5.2 of Kevin Murphy's book.