Lecture 2: Supervised Learning

Tao LIN

February 22, 2023

WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

Feedback on the Questionnaire

- Course Project evaluation protocol
  - CS student: either (by-team) or (by-team-and-supervisor)
  - non-CS student: (by-team-and-supervisor)

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- Theoretical foundation
  - We will explain the mathematical intuitions and insights behind DL methods.

This lecture:

- Basic concept of regression and classification
- Linear regression
    - Definition
    - Gradient Descent (GD) optimization
    - Closed-form Least Square (Geometric and probabilistic interpretation)

Next lecture:

- Overfitting and underftting
- Polynomial regression and Ridge regression
- Model selection
- Bias-Variance Decomposition

Reading materials

- Chapter 1, Stanford CS 229 Lecture Notes,
  `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Chapter 3.1, Bishop, Pattern Recognition and Machine Learning

Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

Table of Contents

1 Regression and Classification
- Regression
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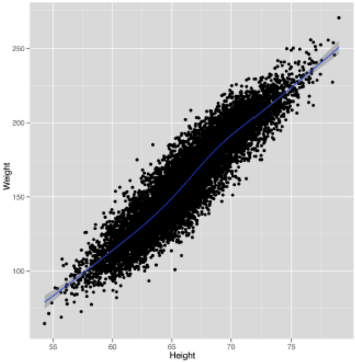
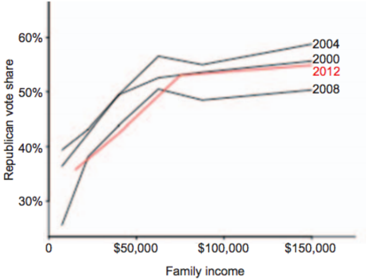
2 Linear Regression
- Definition of Linear Regression
- Optimization and Gradient Descent (GD)
- Normal Equations and Least Squares
- Least Squares Probabilistic Interpretation

What is regression?



(a) Height is correlated with weight. Taken from “Machine Learning for Hackers"



(b) Do rich people vote for republicans? Taken from Avi Feller et. al. 2013, Red state/blue state in 2012 elections.

Regression is to relate input variables to the output variable.

Dataset for regression

In regression:

$$\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y} \tag{1}$$

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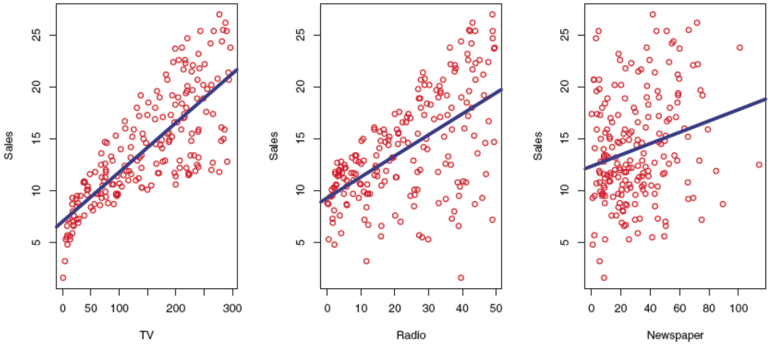

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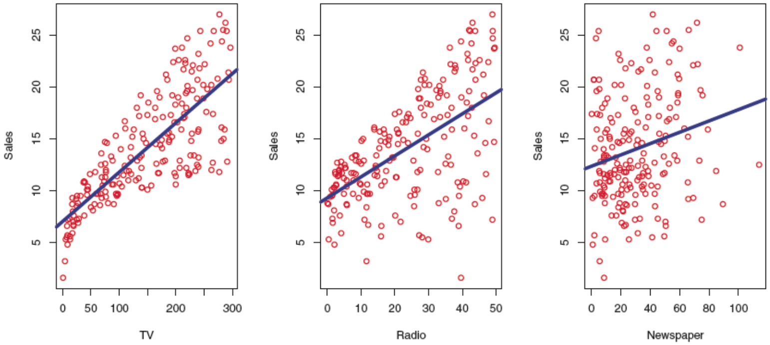

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- The number of pairs N is the data-size and D is the dimensionality.

Two goals of regression

The regression function approximates the output "well enough" given inputs.

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Remark 1 (Correlation $\neq$ Causation)

Regression finds correlation not a causal relationship, so interpret your results with caution.

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Classification

We observe some data

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Remark 2

no ordering between classes.

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Definition

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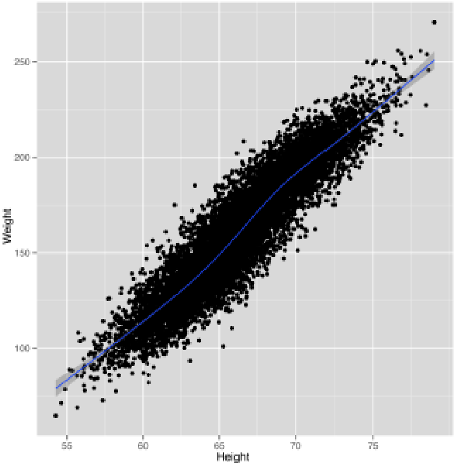

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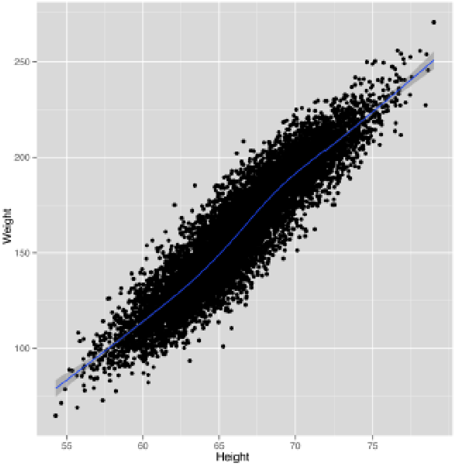

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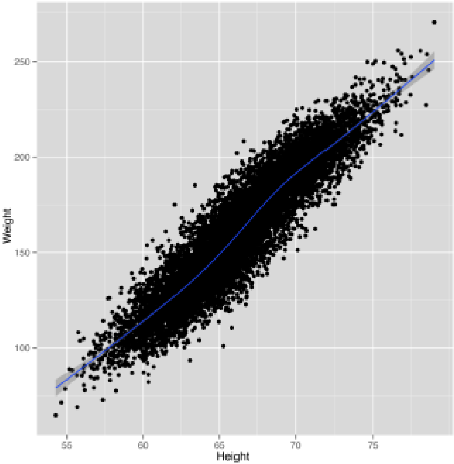
- $y_n \approx f(\mathbf{x}_n)$ for all n and $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y}$
- a linear relationship is assumed for f



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- simple
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- most widely used
- easily generalized to non-linear models
- we can learn almost all fundamental concepts of ML with regression alone

Simple linear regression (w/ only one input dimension):

$$y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1}$$

Here, $\mathbf{w} = (w_0, w_1)$ are the two parameters of the model. They describe f.

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Multiple linear regression (multiple input dimension):

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Given data $\mathcal{D}$, we would like to find $\tilde{\mathbf{w}} = [w_0, w_1, \ldots, w_D]$.

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We need an optimization algorithm!

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A: Optimizing the **cost function** (or energy, loss, training objective) to quantify how well the learned parameter does

Two desirable properties of cost functions

- the cost is symmetric around 0 (penalize positive and negative errors equally)
- the cost penalizes "large" mistakes and "very-large" mistakes similarly

Mean Squared Error (MSE) and Outliers

$$\text{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}\left[y_n - f_{\mathbf{w}}(\mathbf{x}_n)\right]^2 \tag{7}$$

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Definition 3 (Outliers)

Outliers are data examples that are far away from most of the other examples.

MSE is not a good cost function when outliers are present.

- **Pros:** It ensures that *trained model has no outlier predictions with huge errors*.
- **Cons:** It is very sensitive to outliers.

Mean Absolute Error (MAE)

Handling outliers well is a desired *statistical* property.

$$\text{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N} |y_n - f_{\mathbf{w}}(\mathbf{x}_n)| \tag{8}$$

+ MAE is more robust to outliers.
– MAE is not differentiable at zero.

Learning / Estimation / Fitting

Definition 4 (*Learning* problem can be formulated as optimization problem)

Given a cost function $\mathcal{L}(\mathbf{w})$, we wish to find $\mathbf{w}^\star$ which minimizes the cost:

$$\min_{\mathbf{w}} \; \mathcal{L}(\mathbf{w}) \quad \text{subject to } \mathbf{w} \in \mathbb{R}^D \tag{9}$$

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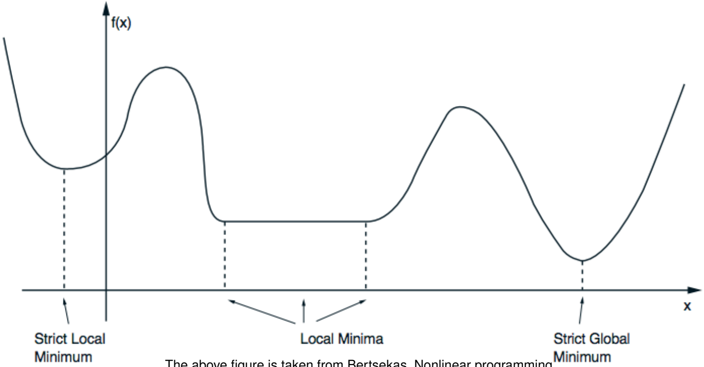
We will use an optimization algorithm to solve the problem (to find a good $\mathbf{w}$).

Optimization Landscapes



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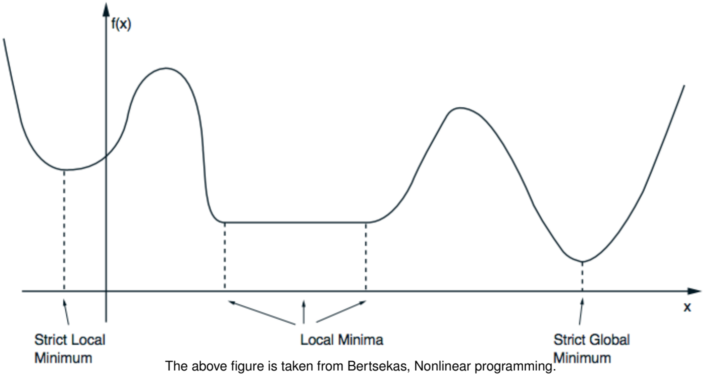

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- A vector $\mathbf{w}^\star$ is a local minimum of $\mathcal{L}$ if it is no worse than its neighbors; i.e. there exists an $\epsilon > 0$ such that,

$$\mathcal{L}(\mathbf{w}^\star) \leq \mathcal{L}(\mathbf{w}), \quad \forall \mathbf{w} \text{ with } \|\mathbf{w} - \mathbf{w}^\star\| < \epsilon$$

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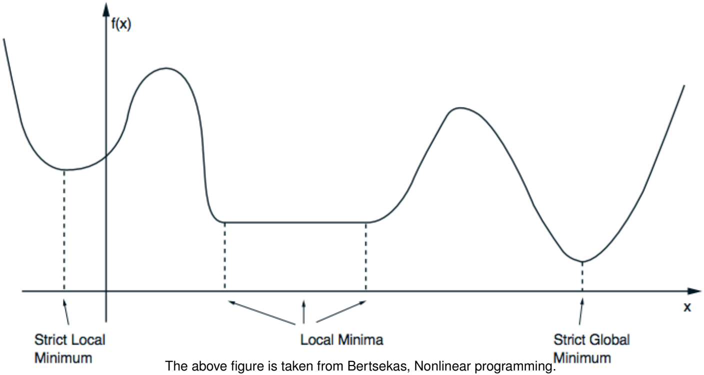

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Smooth Optimization: Follow the Gradient

Definition 5 (Gradient)

A gradient $\nabla\mathcal{L}(\mathbf{w})$ (at a point) is the slope of the ***tangent*** to the function (at that point):

$$\nabla\mathcal{L}(\mathbf{w}) := \left[\frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_1}, \ldots, \frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_D}\right]^\top \in \mathbb{R}^D\,, \tag{10}$$

where it points to the direction of largest increase of the function.

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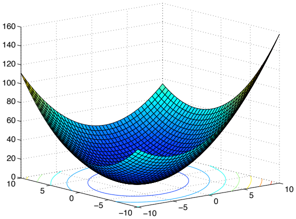
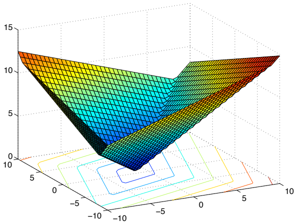
For a 2-parameter model, MSE$(\mathbf{w})$ and MAE$(\mathbf{w})$ are shown below.

(We used $\mathbf{y}_n \approx w_0 + w_1 x_{n1}$ with $\mathbf{y}^\top = [2, -1, 1.5]$ and $\mathbf{x}^\top = [-1, 1, -1]$).





Gradient Descent

Definition 6 (Gradient Descent)

To minimize the cost function, we iteratively take a step in the (opposite) direction of the gradient

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma \nabla \mathcal{L}(\mathbf{w}^{(t)}) \tag{11}$$

where $\gamma > 0$ is the step-size (or learning rate). Then repeat with the next t.

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Gradient Descent for Linear Regression with MSE

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{12}$$

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We define the error vector $\mathbf{e}$:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{13}$$

where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$.

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where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$. The MSE is defined as:

$$\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w} \right)^2 = \tfrac{1}{2N} \mathbf{e}^\top \mathbf{e}, \tag{14}$$

Gradient Descent for Linear Regression with MSE

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \tag{12}$$

We define the error vector $\mathbf{e}$:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N, \tag{13}$$

where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$. The MSE is defined as:

$$\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w} \right)^2 = \tfrac{1}{2N} \mathbf{e}^\top \mathbf{e}, \tag{14}$$

and then the gradient is given by

$$\nabla \mathcal{L}(\mathbf{w}) = -\tfrac{1}{N} \mathbf{X}^\top \mathbf{e} \tag{15}$$

Table of Contents

1. Regression and Classification
   - Regression
   - Classification

2. Linear Regression
   - Definition of Linear Regression
   - Optimization and Gradient Descent (GD)
   - Normal Equations and Least Squares
   - Least Squares Probabilistic Interpretation

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- Linear regression using a mean-squared error cost function is one such case.
- Here its solution can be obtained explicitly, by solving a linear system of equations.

$\Rightarrow$ These equations are sometimes called the normal equations.

$\Rightarrow$ Solving the normal equations is called the least squares.

Recall that the cost function for linear regression with mean-squared error is given by

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N} (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w}), \tag{16}$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D}. \tag{17}$$

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Definition 7 (Convexity)

A function $h(\mathbf{u})$ with $\mathbf{u} \in \mathbb{R}^D$ is convex, if for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^D$ and for any $0 \le \lambda \le 1$, we have:

$$h\left(\lambda \mathbf{u} + (1-\lambda)\mathbf{v}\right) \le \lambda h(\mathbf{u}) + (1-\lambda) h(\mathbf{v}) \tag{19}$$

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Way 1. Recall the definition of $\mathcal{L}$, where

$$\mathcal{L} := \frac{1}{2N} \sum_{n=1}^{N} \left(\mathcal{L}_n := y_n - \mathbf{x}_n^\top \mathbf{w} \right)^2 \,, \tag{20}$$

where each $\mathcal{L}_n$ is the composition of a linear function with a convex function.
$\Rightarrow$ We conclude the proof by “the sum of convex functions is still a convex function”.

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Way 2. By verifying the definition of convexity, that for any $\lambda \in [0, 1]$ and $\mathbf{w}, \mathbf{w}'$,

$$\mathcal{L}(\lambda \mathbf{w} + (1-\lambda)\mathbf{w}') - (\lambda \mathcal{L}(\mathbf{w}) + (1-\lambda)\mathcal{L}(\mathbf{w}')) \leq 0 \,. \tag{21}$$

The LHS of our case $-\frac{1}{2N}\lambda(1-\lambda) \left\|\mathbf{X}(\mathbf{w} - \mathbf{w}')\right\|_2^2$ indeed is non-positive.

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Way 3: check the second derivative (the Hessian) and show that it is positive semi-definite (all its eigenvalues are non-negative).
$\Rightarrow$ the Hessian has the form $\frac{1}{N}\mathbf{X}^\top\mathbf{X}$, which is indeed positive semi-definite (its non-zero eigenvalues are the squares of the non-zero singular values of the matrix $\mathbf{X}$).

Derivation (step 2): finding the minimum of a convex function

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

$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N}\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}). \tag{22}$$

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Given the property of convexity $\nabla\mathcal{L}(\mathbf{w}^\star) = \mathbf{0}$, we can get the normal equations for linear regression:

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}\,, \tag{23}$$

where the error $\mathbf{e} := \mathbf{y} - \mathbf{X}\mathbf{w}$ is orthogonal to all columns of $\mathbf{X}$.

Geometric Interpretation

Definition 8 (Span of a set of vectors)

The **span** of a set of vectors, $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$, is the set of all possible linear combinations of these vectors; i.e. $\text{span}\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} = \{\alpha_1\mathbf{x}_1 + \ldots + \alpha_k\mathbf{x}_k \mid \alpha_1, \ldots, \alpha_k \in \mathbb{R}\}$.

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- The span of $\mathbf{X} \in \mathbb{R}^{N\times D}$ is the space spanned by the columns of $\mathbf{X}$

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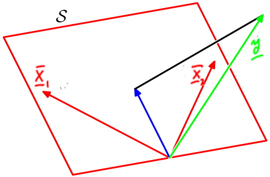

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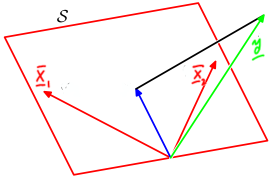

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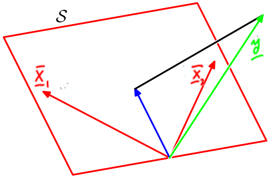

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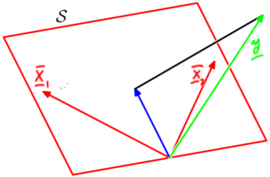

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- the optimum choice for $\mathbf{u}$, i.e. $\mathbf{u}^\star$, requires $\mathbf{y} - \mathbf{u}^\star$ to be orthogonal to $span(\mathbf{X})$.
- $\mathbf{u}^\star$ should be equal to *the projection of* $\mathbf{y}$ *onto* $span(\mathbf{X})$.

Least Squares

We need to solve the linear system of the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, where

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If the Gram matrix is invertible, we can multiply the normal equation by the inverse of the Gram matrix from the left to get a closed-form expression for the minimum:

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

$$\hat{y}_m := \mathbf{x}_m^\top \mathbf{w}^\star = \mathbf{x}_m^\top (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{y}. \tag{25}$$

Invertibility and Uniqueness

Remark 10

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 $\mathbf{X}\mathbf{u} = \mathbf{0}$. It follows that $\mathbf{X}^\top \mathbf{X}\mathbf{u} = \mathbf{0}$, 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 $\mathbf{X}^\top \mathbf{X}\mathbf{v} = \mathbf{0}$. It follows that

$$\mathbf{0} = \mathbf{v}^\top \mathbf{X}^\top \mathbf{X}\mathbf{v} = (\mathbf{X}\mathbf{v})^\top (\mathbf{X}\mathbf{v}) = \|\mathbf{X}\mathbf{v}\|^2 . \tag{26}$$

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

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Can we solve least squares if $\mathbf{X}$ is rank deficient?
Yes, using a linear system solver, e.g., $\text{np.linalg.solve}(\mathbf{X}, \mathbf{y})$.

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Recall: Gaussian distribution and independence

Definition 11 (A Gaussian random variable)

The definition of a Gaussian random variable in $\mathbb{R}$ with mean μ and variance σ^2. It has a density of

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Two random variables X and Y are called *independent* when $p(x, y) = p(x)p(y)$.

A probabilistic model for least-squares

Definition 13 (Data generation process)

We assume that the data is generated by the model,

$$y_n = \mathbf{x}_n^\top \mathbf{w} + \epsilon_n, \tag{29}$$

where

- the ϵ_n (the noise) is a zero-mean Gaussian random variable with variance σ^2
- the noise is independent of each other, and independent of the input.
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The likelihood of the data vector $\mathbf{y} = (y_1, \cdots, y_N)$ given the input $\mathbf{X}$ and the model $\mathbf{w}$ is

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The probabilistic view point: maximize this likelihood over the choice of model $\mathbf{w}$.

Maximum-likelihood estimator (MLE)

Instead of maximizing the likelihood, we can maximize take the logarithm of the likelihood, i.e., log-likelihood (LL):

$$\mathcal{L}_{\mathsf{LL}}(\mathbf{w}) := \log p(\mathbf{y} \,|\, \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst.} \tag{31}$$

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Maximizing the LL is equivalent to minimizing the MSE:

$$\arg\min_{\mathbf{w}} \mathcal{L}_{\text{MSE}}(\mathbf{w}) = \arg\max_{\mathbf{w}} \mathcal{L}_{\text{LL}}(\mathbf{w}). \tag{34}$$

Properties of MLE

MLE is a *sample* approximation to the *expected log-likelihood*:

$$\mathcal{L}_{\mathsf{LL}}(\mathbf{w}) \approx \mathbb{E}_{p(y,\mathbf{x})}\left[\log p(y \mid \mathbf{x}, \mathbf{w})\right] \tag{35}$$

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$$\mathbf{w}_{\text{MLE}} \quad \longrightarrow^{p} \quad \mathbf{w}_{\text{true}} \qquad \text{in probability} \tag{36}$$

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3. The MLE is asymptotically normal, i.e.,

$$(\mathbf{w}_{\text{MLE}} - \mathbf{w}_{\text{true}}) \xrightarrow{d} \frac{1}{\sqrt{N}}\mathcal{N}(\mathbf{w}_{\text{MLE}} \mid \mathbf{0}, \mathbf{F}^{-1}(\mathbf{w}_{\text{true}})), \tag{37}$$

   where $\mathbf{F}(\mathbf{w}) = -\mathbb{E}_{p(\mathbf{y})}\left[\frac{\partial^2 \mathcal{L}}{\partial \mathbf{w} \partial \mathbf{w}^\top}\right]$ is the Fisher information.

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4. MLE is efficient, i.e. it achieves the Cramer-Rao lower bound.

$$\mathrm{Covariance}(\mathbf{w}_{\mathrm{MLE}}) = \mathbf{F}^{-1}(\mathbf{w}_{\mathrm{true}}) \tag{38}$$

Another example

What if we replace Gaussian distribution by a Laplace distribution?

$$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b}\left|y_n - \mathbf{x}_n^\top \mathbf{w}\right|} \tag{39}$$

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we can recover MAE cost function!