Lecture 2: Supervised Learning

Tao LIN

March 1, 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 for DL
  - 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
  - Least Square
  - The probabilistic interpretation of linear regression

Next lecture:

- Over-fitting and under-fitting
- 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`

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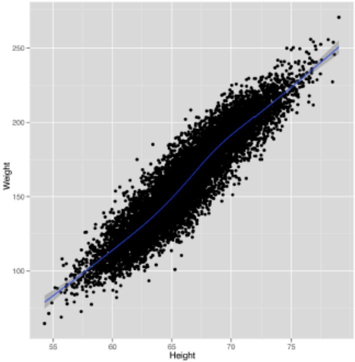
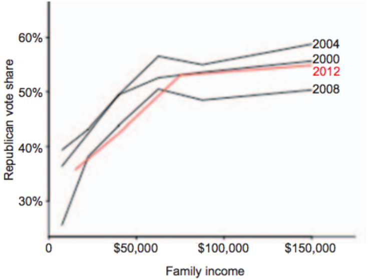
What is regression?



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



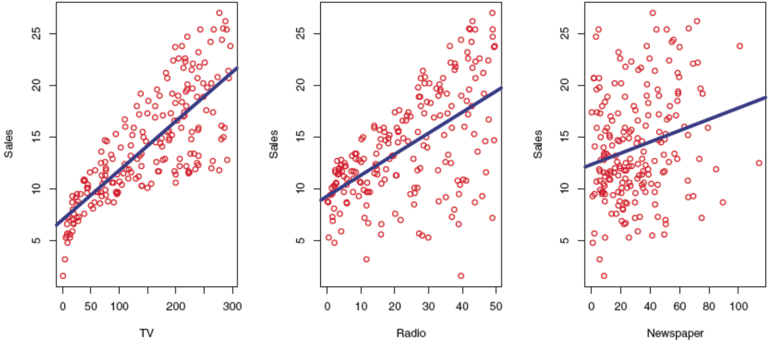
(b) Do rich people vote for republicans? Taken from Avi Feller et. al. 2013, Red state/blue state in 2012 elections.

Regression is to relate input variables to the output variable.

Dataset for regression

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

- data consists of pairs $(\mathbf{x}_n, y_n)$, where y_n is the n'th output and $\mathbf{x}_n$ is a vector of D inputs.



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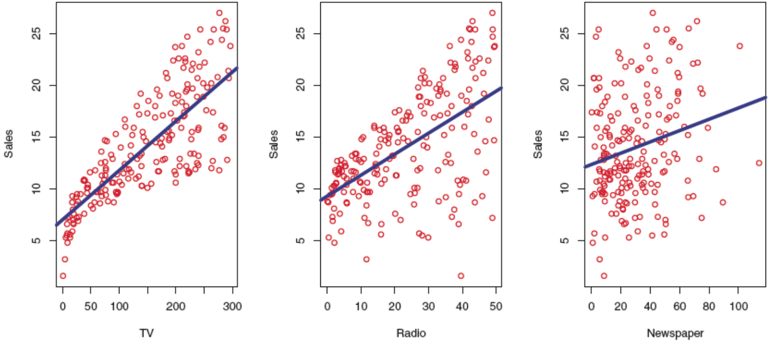
- The number of pairs N is the data-size and D is the dimensionality.



Two goals of regression

The regression function approximates the output y_n "well enough" given inputs $\mathbf{x}_n$.

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   e.g., what is the weight of a person who is 170 cm tall?

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

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Remark 2 (Shortcut learning in Deep Learning)

Models may only learn spurious correlation (and thus sensitive to distribution shifts).

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We observe some data

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Remark 3

no ordering between classes.

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Definition

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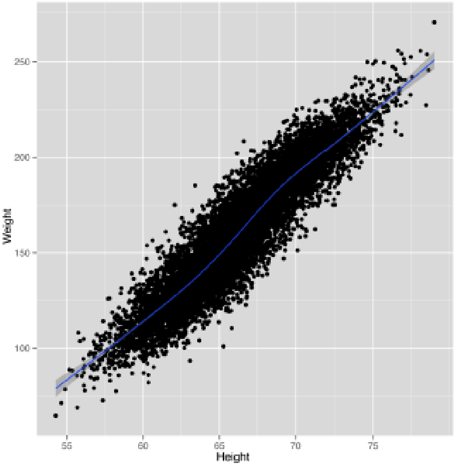

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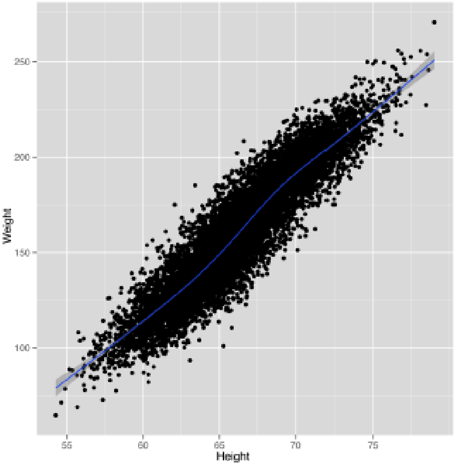

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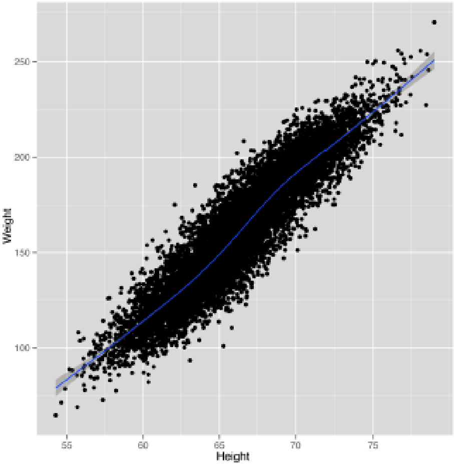
- $y_n \approx f(\mathbf{x}_n)$ for all n and $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y}$
- a linear relationship is assumed for f



Detailed definition

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

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

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We need an optimization algorithm!

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

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Consider the following models.

$$\text{1-parameter model: } y_n \approx w_0$$
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+ MAE is more robust to outliers.
– MAE is not differentiable at zero.

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

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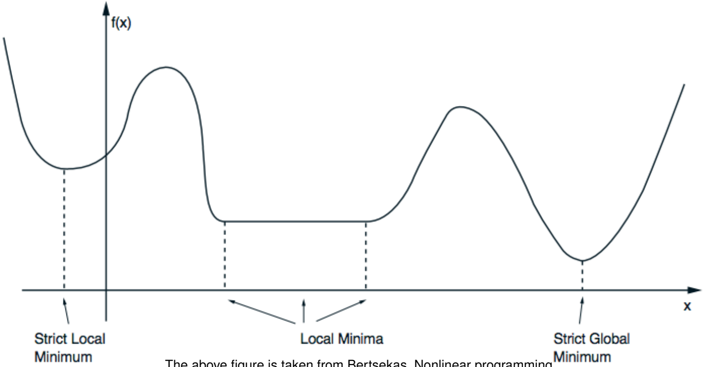
We will use an optimization algorithm to solve the problem (to find a good $\mathbf{w}$).

Optimization Landscapes



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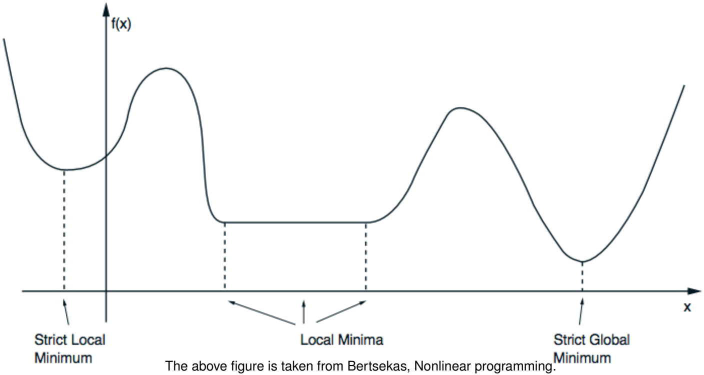

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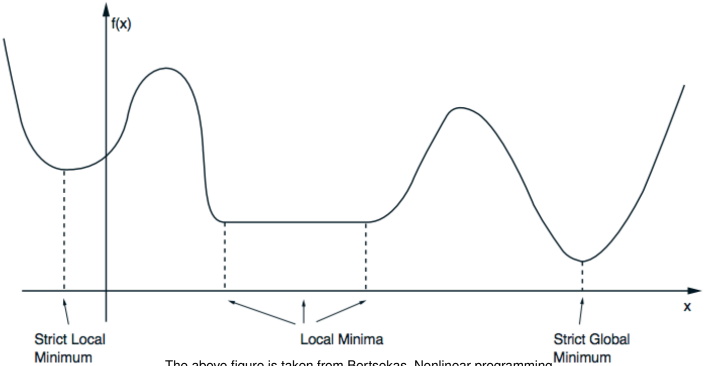

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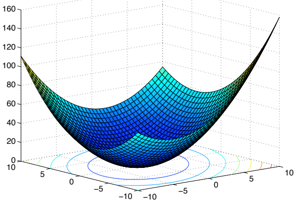
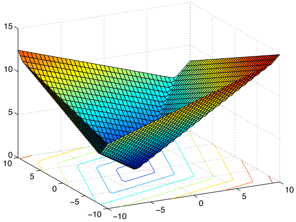
where it points to the direction of the largest increase of the function.

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 $\mathbf{x}^\top = [-1, 1, -1]$).





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

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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.

Gradient Descent for Linear Regression with MSE

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

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

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

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and then the gradient is given by

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- 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 MSE is given by

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

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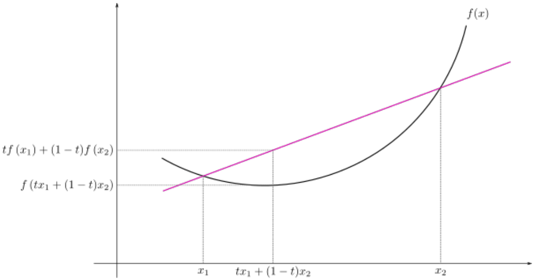
Definition 8 (Convexity)

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 $0 \leq \lambda \leq 1$, we have:

$$h\left(\lambda \mathbf{u} + (1-\lambda)\mathbf{v}\right) \leq \lambda h(\mathbf{u}) + (1-\lambda) h(\mathbf{v}) \tag{18}$$



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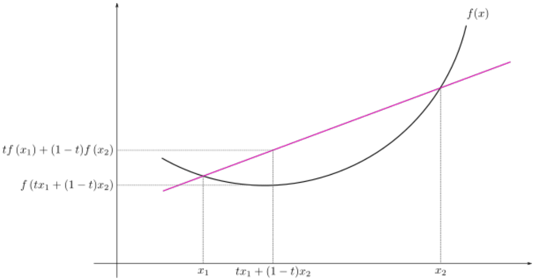

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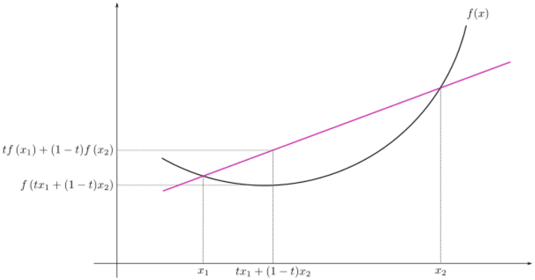

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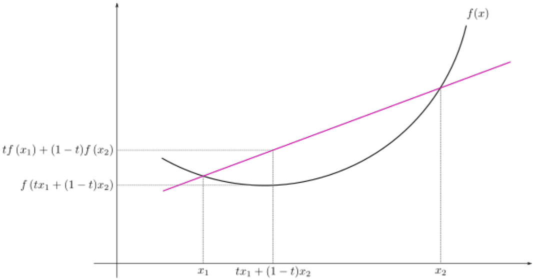

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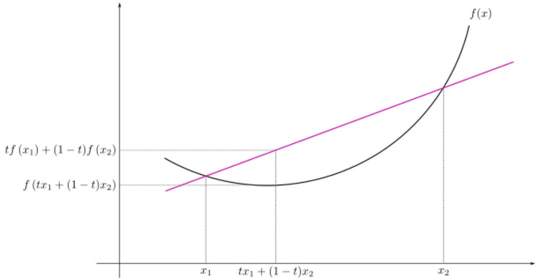

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$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \tag{19}$$

where $\mathbf{w}^\star$ corresponds to the parameter at the optimum point.

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$\Rightarrow$ 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 $\mathbf{X}$).

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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

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

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

Geometric Interpretation

Definition 9 (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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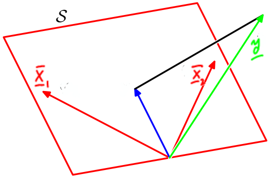

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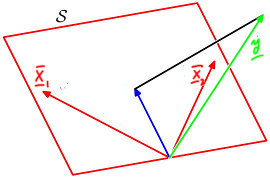

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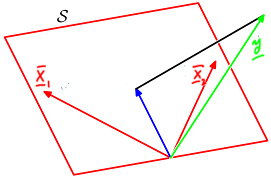

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From $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, we have:

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

Geometric Interpretation

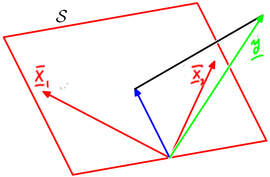
Definition 9 (Span of a set of vectors)

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. span$\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} = \{\alpha_1\mathbf{x}_1 + \ldots + \alpha_k\mathbf{x}_k \,|\, \alpha_1, \ldots, \alpha_k \in \mathbb{R}\}$.

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

$$\mathcal{S} := span(\mathbf{X}) = \{\mathbf{u} := \mathbf{X}\mathbf{w} | \mathbf{w} \in \mathbb{R}^D\}$$

Which element $\mathbf{u}$ of $span(\mathbf{X})$ shall we take? (for the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$)



(taken from Bishop's book)

From $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, we have:

- 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

$$\mathbf{X}^\top y = \underbrace{\mathbf{X}^\top\mathbf{X}}_{\text{Gram matrix}} \mathbf{w} \tag{24}$$

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

$$\hat{y}_m := \mathbf{x}_m^\top\mathbf{w}^\star = \mathbf{x}_m^\top(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}. \tag{26}$$

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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* $rank(\mathbf{X}) = D$.

Rank Deficiency and Ill-Conditioning

Unfortunately, in practice, $\mathbf{X} \in \mathbb{R}^{N \times D}$ is often rank deficient.

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

Table of Contents

Recall: Gaussian distribution and independence

Definition 11 (A Gaussian random variable)

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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 linear regression

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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 the negative of the log-likelihood, i.e., log-likelihood (LL):

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

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

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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 the Gaussian distribution with 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 the MAE cost function!

This lecture:

- Basic concept of regression and classification
- Linear regression
    - Definition
    - Gradient Descent (GD) optimization
    - Least Square
    - The probabilistic interpretation of Linear Regression

Next lecture:

- Over-fitting and under-fitting
- Polynomial regression and Ridge regression
- Model selection
- Bias-Variance Decomposition