Maximum Likelihood Estimation (MLE) Regularizations

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Maths for Computer Science, Fall 2021

References

The contents of this document are taken mainly from the follow sources:

- Kevin P. Murphy. Probabilistic Machine Learning: An Introduction. [1]

[1] https://probml.github.io/pml-book/book1.html

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Introduction

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  where $\mathcal{L}(\boldsymbol{\theta})$ is some kind of loss function or objective function.
- The process of quantifying uncertainty about an unknown quantity estimated from a finite sample of data is called **inference**.
- In deep learning, the term "inference" refers to "prediction", namely computing

$$p(y|x, \hat{\boldsymbol{\theta}})$$

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Maximum Likelihood Estimation

- The most common approach to parameter estimation is to pick the parameters that assign the highest probability to the training data. This is called **maximum likelihood estimation** or **MLE**.

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- We usually assume the training examples are "independent and identically distributed", and are sampled from the same distribution (i.e., the **iid** assumption). The conditional likelihood becomes

$$p(\mathcal{D}|\boldsymbol{\theta}) = p(y_1, y_2, \ldots, y_N | x_1, x_2, \ldots, x_N, \boldsymbol{\theta}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta})$$

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- We usually work with the **log likelihood**, which decomposes into a sum of terms, one per example.

$$\mathrm{LL}(\boldsymbol{\theta}) = \log p(\mathcal{D}|\boldsymbol{\theta}) = \log \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta}) = \sum_{n=1}^{N} \log p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta})$$

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- Minimizing this will give the MLE.

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Bernoulli Random Variables

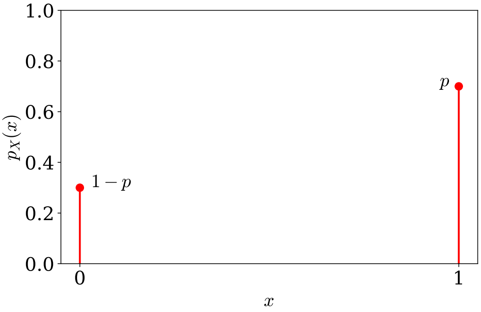
- A Bernoulli r.v. X takes two possible values, usually 0 and 1, modeling random experiments that have two possible outcomes (e.g., "success" and "failure").
  - e.g., tossing a coin. The outcome is either Head or Tail.
  - e.g., taking an exam. The result is either Pass or Fail.
  - e.g., classifying images. An image is either Cat or Non-cat.

Bernoulli Random Variables

Definition

A random variable X is a Bernoulli random variable with parameter $p \in [0, 1]$, written as $X \sim Bernoulli(p)$ if its PMF is given by

$$P_X(x) = \begin{cases} p, & \text{for } x = 1 \\ 1 - p, & \text{for } x = 0. \end{cases}$$



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- After doing the experiment, the following values for X_i's are observed: $x_1 = 1, x_2 = 0, x_3 = 1, x_4 = 1$.
- Note that X_i's are i.i.d. (independent and identically distributed) and $X_i \sim Bernoulli(\frac{\theta}{3})$. For which value of θ is the probability of the observed sample is the largest?

Example

$$P_{X_i}(x) = \begin{cases} \frac{\theta}{3}, & \text{for } x = 1 \\ 1 - \frac{\theta}{3}, & \text{for } x = 0 \end{cases}$$

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X_i's are independent, the joint PMF of X_1, X_2, X_3, X_4 can be written

$$P_{X_1X_2X_3X_4}(x_1, x_2, x_3, x_4) = P_{X_1}(x_1)P_{X_2}(x_2)P_{X_3}(x_3)P_{X_4}(x_4)$$

$$P_{X_1X_2X_3X_4}(1, 0, 1, 1) = \frac{\theta}{3} \cdot \left(1 - \frac{\theta}{3}\right) \cdot \frac{\theta}{3} \cdot \frac{\theta}{3} = \left(\frac{\theta}{3}\right)^3 \left(1 - \frac{\theta}{3}\right)$$

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θ	$P_{X_1X_2X_3X_4}(1,0,1,1;\theta)$
0	0
1	0.0247
2	0.0988
3	0

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The observed data is most likely to occur for $\theta = 2$.
We may choose $\hat{\theta} = 2$ as our estimate of θ.

MLE for the Bernoulli distribution

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- The probability distribution for this rv is the Bernoulli. The NLL for the Bernoulli distribution is

$$\begin{aligned}\mathtt{NLL}(\theta) &= -\log \prod_{n=1}^{N} p(y_n|\theta) = -\log \prod_{n=1}^{N} \theta^{\mathbb{I}(y_n=1)}(1-\theta)^{\mathbb{I}(y_n=0)} \\ &= -\sum_{n=1}^{N} \mathbb{I}(y_n = 1)\log\theta + \mathbb{I}(y_n = 0)\log(1-\theta) \\ &= -[N_1 \log\theta + N_0 \log(1-\theta)]\end{aligned}$$

where $N_1 = \sum_{n=1}^{N} \mathbb{I}(y_n = 1)$ is the number of heads, and $N_0 = \sum_{n=1}^{N} \mathbb{I}(y_n = 0)$ is the number of tails.

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- $N = N_0 + N_1$ is the **sample size**.

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$$\texttt{NLL}(\theta) = -[N_1 \log \theta + N_0 \log(1-\theta)]$$

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- The MLE is given by

$$\hat{\theta}_{\texttt{mle}} = \frac{N_1}{N_0 + N_1}$$

which is the empirical fraction of heads.

MLE for the categorical distribution

- Suppose we roll a K-sided dice N times.
- Let $Y_n \in \{1, \ldots, K\}$ be the n-th outcome, where $Y_n \sim \texttt{Cat}(\boldsymbol{\theta})$.
- We want to estimate $\boldsymbol{\theta}$ from the dataset $\mathcal{D}\{y_n : n = 1 : N\}$.

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- The compute the MLE, we have to minimize the NLL subject to the **constraint** that

$$\sum_{k=1}^{K} \theta_k = 1$$

MLE for the categorical distribution

- We use the method of Lagrange multipliers. The Lagrangian is as

$$\mathcal{L}(\boldsymbol{\theta}, \lambda) = -\sum_k N_k \log \theta_k - \lambda\left(1 - \sum_k \theta_k\right)$$

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- We can solve for λ using the sum-to-one constraint

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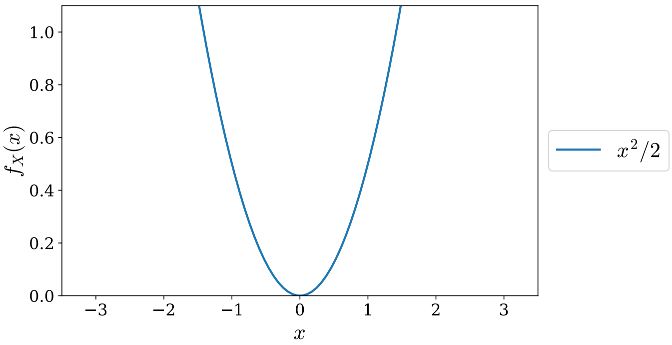
- Thus the MLE is given by $\hat{\theta}_k = \frac{N_k}{\lambda} = \frac{N_k}{N}$, the empirical fraction of times event k occurs.

Standard Normal (Gaussian) Random Variable $N(0, 1)$



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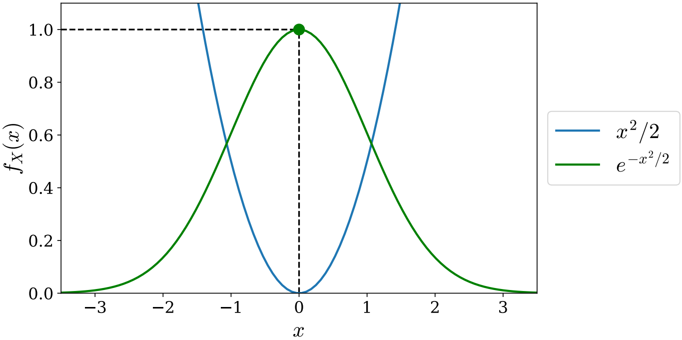

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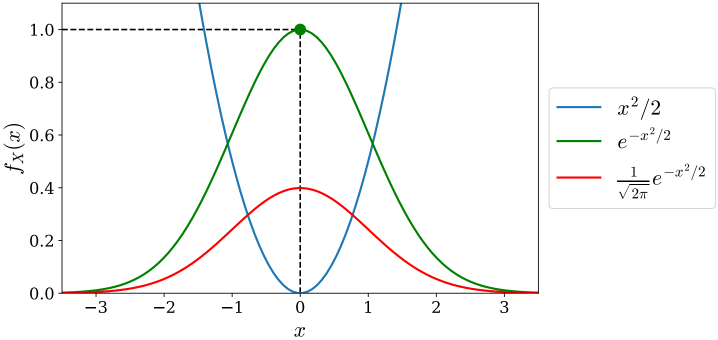
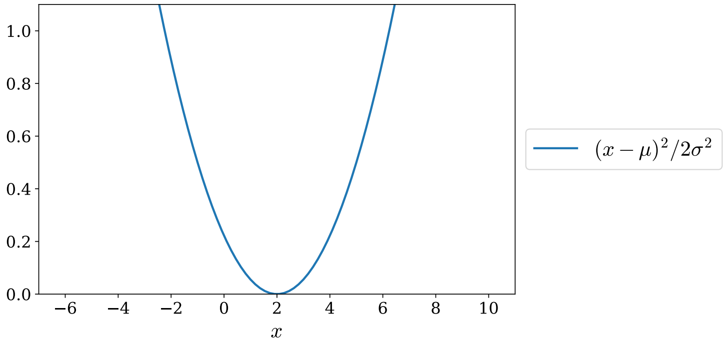


$$\int_{-\infty}^{\infty} e^{-x^2/2}\, dx = \sqrt{2\pi}$$

$$f_X(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

General Normal (Gaussian) Random Variable $N(\mu, \sigma^2)$



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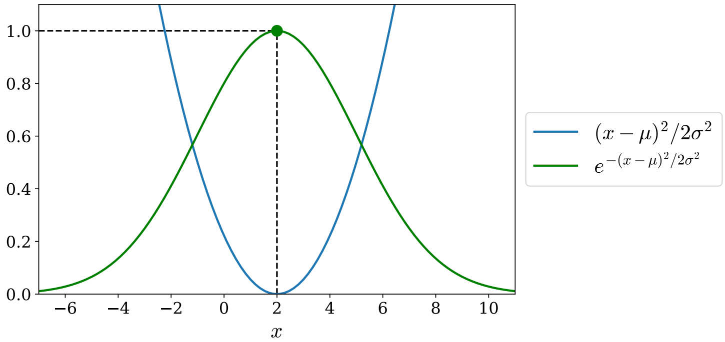

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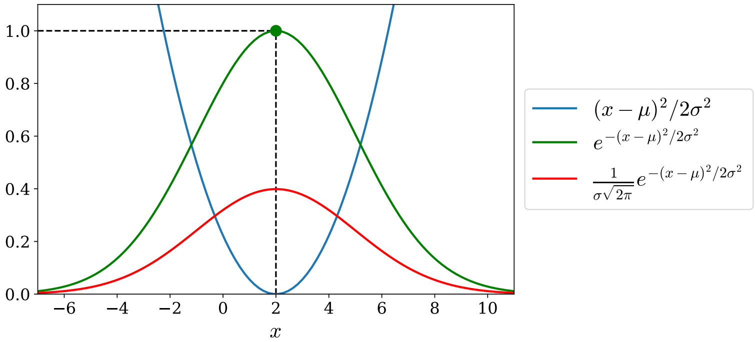

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$
$$= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2\right)$$
$$\mathrm{E}[X] = \mu \qquad \mathrm{Var}(X) = \sigma^2$$

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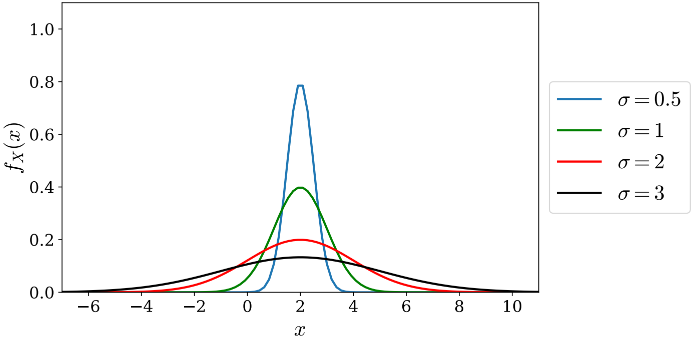

- Smaller σ, narrower PDF.
- Let $Y = aX + b \qquad N \sim N(\mu, \sigma^2)$
- Then, $\mathrm{E}[Y] = aE[X] + b \qquad \mathrm{Var}(Y) = a^2\sigma^2$ (always true)
- But also, $Y \sim N(a\mu + b, a^2\sigma^2)$

Example

- We have $N = 3$ data points $y_1 = 1,\ y_2 = 0.5,\ y_3 = 1.5$ which are independent and Gaussian with unknown mean μ and variance 1:

$$y_i \sim \mathcal{N}(\mu, 1)$$

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- Consider two guesses $\mu = 1.0$ and $\mu = 2.5$. Which has higher likelihood?
- Finding the μ that maximizes the likelihood is equivalent to moving the Gaussian until the product $P(y_1|\mu)P(y_2|\mu)P(y_3|\mu)$ is maximized.

MLE for the univariate Gaussian

- $Y \sim \mathcal{N}(\mu, \sigma^2)$ and $\mathcal{D} = \{y_n : n = 1 : N\}$ be an iid sample of size N.

$$p(y|\theta) = \mathcal{N}(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2 \right)$$

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- We can estimate the parameters $\boldsymbol{\theta} = (\mu, \sigma^2)$ using MLE.
- We derive the NLL, which is given by

$$\begin{aligned}\mathtt{NLL}(\mu, \sigma^2) &= -\sum_{n=1}^{N} \log\left[\left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(y_n-\mu)^2\right)\right] \\ &= \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n-\mu)^2 + \frac{N}{2}\log(2\pi\sigma^2)\end{aligned}$$

MLE for the univariate Gaussian

- $Y \sim \mathcal{N}(\mu, \sigma^2)$ and $\mathcal{D} = \{y_n : n = 1 : N\}$ be an iid sample of size N.

$$p(y|\theta) = \mathcal{N}(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2 \right)$$

- We can estimate the parameters $\boldsymbol{\theta} = (\mu, \sigma^2)$ using MLE.
- We derive the NLL, which is given by

$$\begin{aligned} \mathtt{NLL}(\mu, \sigma^2) &= -\sum_{n=1}^{N} \log\left[\left(\frac{1}{2\pi\sigma^2} \right)^{\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(y_n - \mu)^2 \right) \right] \\ &= \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mu)^2 + \frac{N}{2} \log(2\pi\sigma^2) \end{aligned}$$

- The minimum of this function must satisfy the following conditions

$$\frac{\partial}{\partial \mu} \mathtt{NLL}(\mu, \sigma^2) = 0, \quad \frac{\partial}{\partial \sigma^2} \mathtt{NLL}(\mu, \sigma^2) = 0$$

MLE for the univariate Gaussian

- The solution is given by

$$\hat{\mu}_{\mathtt{mle}} = \frac{1}{N}\sum_{n=1}^{N} y_n = \bar{y}$$

$$\hat{\sigma}^2_{\mathtt{mle}} = \frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{\mu}_{\mathtt{mle}})^2 = \frac{1}{N}\left[\sum_{n=1}^{N} y_n^2 + \hat{\mu}^2_{\mathtt{mle}} - 2y_n\hat{\mu}_{\mathtt{mle}}\right] = s^2 - \bar{y}^2$$

$$s^2 \triangleq \frac{1}{N}\sum_{n=1}^{N} y_n^2$$

- The quantities $\bar{y}$ and s^2 are called the **sufficient statistics** of the data because they are sufficient to compute the MLE.

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- The quantities $\bar{y}$ and s^2 are called the **sufficient statistics** of the data because they are sufficient to compute the MLE.
- Sometimes, we might se the estimate for the variance as

$$\hat{\sigma}^2 = \frac{1}{N-1}\sum_{n=1}^{N}(y_n - \hat{\mu}_{\texttt{mle}})^2$$

which is not the MLE, but is a different kind of estimate.

Table of Contents

MLE for linear regression

- We can make the parameters of the Gaussian to be functions of some input variables

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \mathcal{N}(y|f_\mu(\boldsymbol{x};\boldsymbol{\theta}), f_\sigma(\boldsymbol{x};\boldsymbol{\theta})^2)$$

$f_\mu(\boldsymbol{x};\boldsymbol{\theta}) \in \mathbb{R}$ predicts mean, and $f_\sigma(\boldsymbol{x};\boldsymbol{\theta}) \in \mathbb{R}_+$ predicts variance.

MLE for linear regression

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- It is common to assume that the variance is *fixed*, and is *independent* of the input. This is called **homoscedastic regression**.

MLE for linear regression

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- It is common to assume that the variance is *fixed*, and is *independent* of the input. This is called **homoscedastic regression**.
- Furthermore, it is common to assume the mean is a linear function of the input. The resulting model is called **linear regression**.

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \mathcal{N}(y|\boldsymbol{w}^T\boldsymbol{x} + b, \sigma^2)$$

  where $\boldsymbol{\theta} = (\boldsymbol{w}, b, \sigma)$.

MLE for linear regression

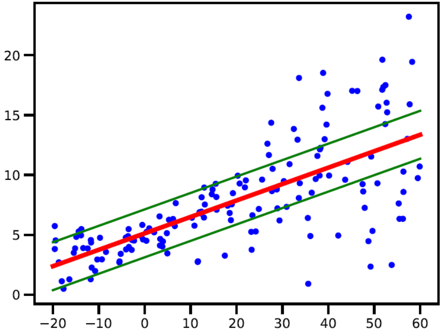

Figure: Linear regression using Gaussian output with mean $\mu(x) = b + wx$ and fixed variance σ^2.

- The figure plots the 95% predictive interval $[\mu(x) - 2\sigma, \mu(x) + 2\sigma]$.
- This is the uncertainty in the predicted *observation* y given x, and capture the variablity in the blue dots.

MLE for linear regression

- Linear regression model

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \mathcal{N}(y|\boldsymbol{w}^T\boldsymbol{x}, \sigma^2)$$

where $\boldsymbol{\theta} = (\boldsymbol{w}, \sigma^2)$, and $\boldsymbol{w} = (b, w_1, w_2, \ldots, w_D)$.

MLE for linear regression

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- Assume that σ^2 is fixed, we estimate the weights $\boldsymbol{w}$. The NLL is

$$\mathtt{NLL}(\boldsymbol{w}) = -\sum_{n=1}^{N} \log\left[\left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}(y_n - \boldsymbol{w}^T\boldsymbol{x}_n)^2\right)\right]$$

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- Dropping the *irrelevant* additive constants gives the simplified objective, known as the **residual sum of squares** or **RSS**:

$$\mathtt{RSS}(\boldsymbol{w}) = \sum_{n=1}^{N}(y_n - \boldsymbol{w}^T\boldsymbol{x}_n)^2 = \sum_{n=1}^{N} r_n^2$$

where r_n is the n-th **residual error**.

MLE for linear regression

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$$\mathtt{RSS}(\boldsymbol{w}) = \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\mathsf{T}\boldsymbol{x}_n)^2$$

MLE for linear regression

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$$\mathtt{RSS}(\boldsymbol{w}) = \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n)^2$$

- **Mean squared error** or **MSE**:

$$\mathtt{MSE}(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n)^2$$

MLE for linear regression

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$$\texttt{RMSE}(\boldsymbol{w}) = \sqrt{\texttt{MSE}(\boldsymbol{w})} = \sqrt{\frac{1}{N} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n)^2}$$

MLE for linear regression

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- We can compute the MLE by minimizing the NLL, RSS, MSE, or RMSE. All give the same results.

MLE for linear regression

- The RSS can be written in matrix notation as follows

$$\mathtt{RSS}(\boldsymbol{w}) = \sum_{n=1}^{N} (y_n - \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n)^2 = \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 = (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^{\mathsf{T}} (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

MLE for linear regression

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- The gradient is given by

$$\nabla_{\boldsymbol{w}} \mathtt{RSS}(\boldsymbol{w}) = \boldsymbol{X}^\mathsf{T} \boldsymbol{X} \boldsymbol{w} - \boldsymbol{X}^\mathsf{T} \boldsymbol{y}$$

MLE for linear regression

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$$\nabla_{\boldsymbol{w}} \text{RSS}(\boldsymbol{w}) = \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^\top \boldsymbol{y}$$

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$$\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} = \boldsymbol{X}^\top \boldsymbol{y}$$

- These are known as the **normal equations**.

MLE for linear regression

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- These are known as the **normal equations**.
- The MLE solution $\hat{\boldsymbol{w}}_{\mathtt{mle}}$ is called the **ordinary least squares (OLS)** solution:

$$\hat{\boldsymbol{w}}_{\mathtt{mle}} = \operatorname*{argmin}_{\boldsymbol{w}} \mathrm{RSS}(\boldsymbol{w}) = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

MLE for linear regression

$$\hat{\boldsymbol{w}}_{\mathtt{mle}} = \underset{\boldsymbol{w}}{\operatorname{argmin}} \, \mathtt{RSS}(\boldsymbol{w}) = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

- The quantity $\boldsymbol{X}^\dagger = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top$ is the (left) pseudo-inverse of the (non-square) matrix $\boldsymbol{X}$.
- Is the solution $\hat{\boldsymbol{w}}_{\mathtt{mle}}$ unique?

MLE for linear regression

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$$\boldsymbol{v}^\top (\boldsymbol{X}^\top \boldsymbol{X}) \boldsymbol{v} = (\boldsymbol{X}\boldsymbol{v})^\top (\boldsymbol{X}\boldsymbol{v}) = \|\boldsymbol{X}\boldsymbol{v}\|^2 > 0$$

MLE for linear regression

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- In the full rank case, the $\texttt{RSS}(\boldsymbol{w})$ has a **unique global minimum**.

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Overfitting

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- The model has enough parameters to perfectly fit the observed training data, so it can perfectly match the empirical distribution.
- In most cases, the empirical distribution is not the same as the true distribution. Putting all the probability mass on the observed set of N examples will not leave over any probability for novel data in the future. The model may not **generalize**.

Example: MLE for Linear Regression

Example 1:

- Training data: $\boldsymbol{x}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ y_1 = 1 \quad \boldsymbol{x}_2 = \begin{bmatrix} 1 \\ \epsilon \end{bmatrix}, \ y_2 = 1.$

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Example 2:

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- Training data: $\boldsymbol{x}_1 = \begin{bmatrix}1\\0\end{bmatrix}$, $y_1 = 1+\epsilon \quad \boldsymbol{x}_2 = \begin{bmatrix}1\\\epsilon\end{bmatrix}$, $y_2 = 1$.
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Solve these 2 examples in 10 MINUTES, and submit on our course website.

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Example: MLE for Linear Regression

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- Training data: $\boldsymbol{x}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $y_1 = 1 + \epsilon$ $\quad \boldsymbol{x}_2 = \begin{bmatrix} 1 \\ \epsilon \end{bmatrix}$, $y_2 = 1$.
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Regularization

- The main solution to overfitting is to use **regularization**.
- We add a penalty term to the NLL (or empirical risk):

$$\mathcal{L}(\boldsymbol{\theta}; \lambda) = \left[\frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(\boldsymbol{x}_n; \boldsymbol{\theta})) \right] + \lambda C(\boldsymbol{\theta})$$

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- If ℓ is the log loss, the regularized objective becomes

$$\mathcal{L}(\boldsymbol{\theta}; \lambda) = -\frac{1}{N} \sum_{n=1}^{N} \log p(y_n | x_n, \boldsymbol{\theta}) - \lambda \log p(\boldsymbol{\theta})$$

Maximum a posteriori estimation (MAP)

$$\mathcal{L}(\boldsymbol{\theta};\lambda) = -\frac{1}{N}\sum_{n=1}^{N}\log p(y_n|x_n,\boldsymbol{\theta}) - \lambda\log p(\boldsymbol{\theta})$$

- By setting $\lambda = 1$ and rescaling $p(\boldsymbol{\theta})$ appropriately, we can equivalently minimize the following

$$\mathcal{L}(\boldsymbol{\theta};\lambda) = -\left[\sum_{n=1}^{N}\log p(y_n|x_n,\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\right] = -[\log p(\mathcal{D}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})]$$

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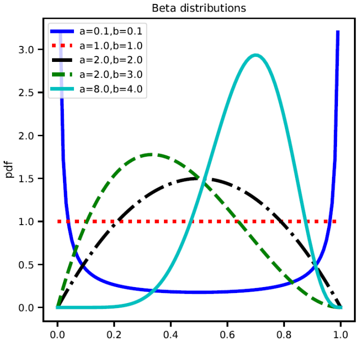
- This is **MAP estimation**, or **maximum a posteriori estimation**.

MAP estimation for Bernoulli distribution

- Coin tossing. If we observe just one head, the MLE is $\hat{\theta}_{\mathtt{mle}} = 1$.
- To avoid this, we can add a penalty to θ to discourage "extreme" values, such as $\theta = 0$ or $\theta = 1$.
- We can use a beta distribution as our prior $p(\theta) = \mathtt{Beta}(\theta|a,b)$, where $a, b > 1$ encourages values of θ near to $a/(a+b)$.



- If $a = b = 1$, we get uniform distribution
- If a and b are both less than 1, we get bimodal distribution.
- If a and b are both greater than 1, the distribution is unimodal.

$$\mathtt{mean} = \frac{a}{a+b}$$

$$\mathtt{var} = \frac{ab}{(a+b)^2(a+b+1)}$$

MAP estimate for Bernoulli dsitribution

- Using the beta distribution as our prior $p(\theta) = \texttt{Beta}(\theta|a, b)$, the log likelihood plus log prior becomes

$$\begin{aligned}\texttt{LL}(\theta) &= \log p(\mathcal{D}|\theta) + \log p(\theta) \\ &= [N_1 \log \theta + N_0 \log(1-\theta)] + [(a-1)\log \theta + (b-1)\log(1-\theta)]\end{aligned}$$

- The MAP estimate is

$$\hat{\theta}_{\texttt{map}} = \frac{N_1 + a - 1}{N_1 + N_0 + a + b - 2}$$

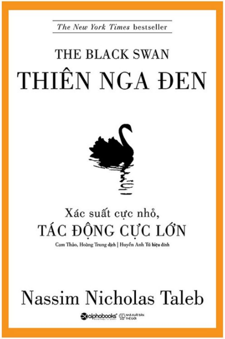
- If we set $a = b = 2$, that weakly favor a value of θ near 0.5, the estimate becomes

$$\hat{\theta}_{\texttt{map}} = \frac{N_1 + 1}{N_1 + N_0 + 2}$$

- This is called **add-one smoothing** to avoid the **zero count problem**.

Black swan paradox

- The zero-count problem, and overfitting, is analogous to the **black swan paradox**.



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- The zero-count problem, and overfitting, is analogous to the **black swan paradox**.
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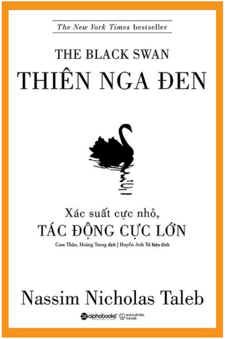

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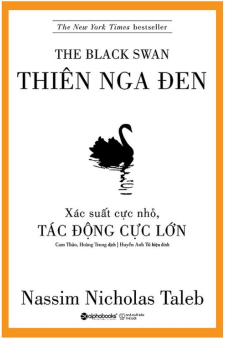

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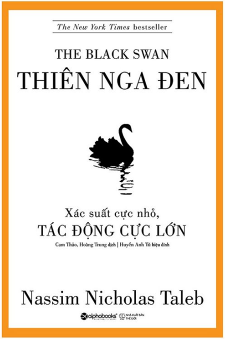
- It is used to illustrate the problem of **induction**: how to draw general conclusions about the future from specific observations from the past.
- The solution to the paradox is to admit that induction is *in general* impossible.
- The best we can do is to make plausible guesses by combining the empirical data with prior knowledge.



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- We use a zero-mean Gaussian prior $p(\boldsymbol{w})$. The MAP estimate is

$$\hat{\boldsymbol{w}}_{\texttt{map}} = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, \texttt{NLL}(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2$$

  where $\|\boldsymbol{w}\|_2^2 = \sum_{d=1}^{D} w_d^2$. We penalize the magnitude of weight vectors $\boldsymbol{w}$, rather than the bias term b.

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- The equation is called ℓ_2 **regularization** or **weight decay**.
- The larger the value of λ, the more the parameters are penalized for being large (i.e., deviating from the zero-mean prior), and thus the less flexible the model.

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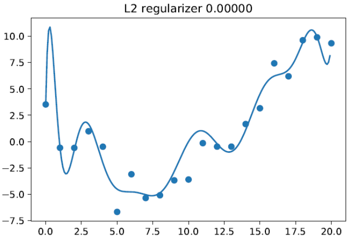
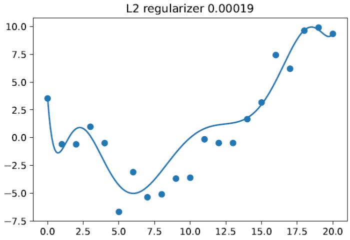
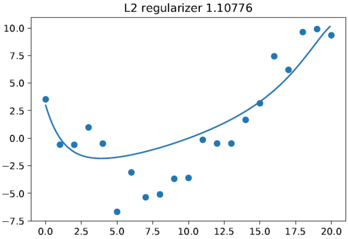
- Increasing λ can reduce overfitting.


L2 regularizer 0.00000
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

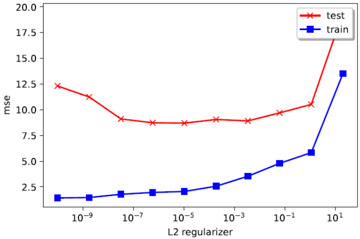
(a)


L2 regularizer 0.00019
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

(b)


L2 regularizer 1.10776
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

(c)


test
train
mse
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
10^{-9}
10^{-7}
10^{-5}
10^{-3}
10^{-1}
10^{1}
L2 regularizer

(d)

Ridge regression

- MAP estimation with a zero-mean Gaussian prior $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|0, \lambda^{-1}\boldsymbol{I})$.

$$\begin{aligned}
\hat{\boldsymbol{w}}_{\texttt{map}} &= \underset{\boldsymbol{w}}{\operatorname{argmin}} \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^\mathsf{T}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) + \frac{1}{2\tau^2}\boldsymbol{w}^\mathsf{T}\boldsymbol{w} \\
&= \underset{\boldsymbol{w}}{\operatorname{argmin}} \operatorname{RSS}(\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_2^2
\end{aligned}$$

where $\lambda = \frac{\sigma^2}{\tau^2}$ is proportional to the strength of the prior, and

$$\|\boldsymbol{w}\|_2 = \sqrt{\sum_{d=1}^{D} |w_d|^2} = \sqrt{\boldsymbol{w}^\mathsf{T}\boldsymbol{w}}$$

is the ℓ_2 norm of the vector $\boldsymbol{w}$.

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  is the ℓ_2 norm of the vector $\boldsymbol{w}$.

- We do not penalize the offset w_0, since that only affects the global mean of the output, and does not contribute to the overfitting.

Ridge Regression

- The MAP estimate corresponds to minimizing the penalized objective:

$$J(\boldsymbol{w}) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^{\mathsf{T}}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_2^2$$

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- Therefore,

$$\begin{aligned}\hat{\boldsymbol{w}}_{\mathtt{map}} &= (\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X} + \lambda\boldsymbol{I}_D)^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{y} \\ &= (\sum_n \boldsymbol{x}_n\boldsymbol{x}_n^{\mathsf{T}} + \lambda\boldsymbol{I}_D)^{\text{-1}}(\sum_n y_n\boldsymbol{x}_n)\end{aligned}$$

Example: MAP for Linear Regression

- Maximum likelihood estimation. Let $\epsilon = 0.1$
- Ex. 1: $\hat{\boldsymbol{w}}_{\texttt{mle}} = \begin{bmatrix} 1 & -1/\epsilon \\ -1/\epsilon & 2/\epsilon^2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$
- Ex. 2: $\hat{\boldsymbol{w}}_{\texttt{mle}} = \begin{bmatrix} 1 & -1/\epsilon \\ -1/\epsilon & 2/\epsilon^2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1+\epsilon \\ 1 \end{bmatrix} = \begin{bmatrix} 1+\epsilon \\ -1 \end{bmatrix} = \begin{bmatrix} 1.1 \\ -1 \end{bmatrix}.$

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- Maximum a posteriori estimation. Let $\lambda = 0.05$

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- Maximum a posteriori estimation. Let $\lambda = 0.05$
- $(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_D) = \begin{bmatrix} 2+\lambda & \epsilon \\ \epsilon & \epsilon^2 + \lambda \end{bmatrix} = \begin{bmatrix} 2.05 & 0.1 \\ 0.1 & 0.06 \end{bmatrix}$

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- $(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_D)^{-1} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix}$

Example: MAP for Linear Regression

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- Ex. 2: $\hat{\boldsymbol{w}}_{\texttt{mle}} = \begin{bmatrix} 1 & -1/\epsilon \\ -1/\epsilon & 2/\epsilon^2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1+\epsilon \\ 1 \end{bmatrix} = \begin{bmatrix} 1+\epsilon \\ -1 \end{bmatrix} = \begin{bmatrix} 1.1 \\ -1 \end{bmatrix}$.
- Maximum a posteriori estimation. Let $\lambda = 0.05$
- $(\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda \boldsymbol{I}_D) = \begin{bmatrix} 2+\lambda & \epsilon \\ \epsilon & \epsilon^2+\lambda \end{bmatrix} = \begin{bmatrix} 2.05 & 0.1 \\ 0.1 & 0.06 \end{bmatrix}$
- $(\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda \boldsymbol{I}_D)^{-1} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix}$
- Ex. 1: $\hat{\boldsymbol{w}}_{\texttt{map}} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.9735 \\ 0.0442 \end{bmatrix}$

Example: MAP for Linear Regression

- Maximum likelihood estimation. Let $\epsilon = 0.1$
- Ex. 1: $\hat{\boldsymbol{w}}_{\texttt{mle}} = \begin{bmatrix} 1 & -1/\epsilon \\ -1/\epsilon & 2/\epsilon^2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$.
- Ex. 2: $\hat{\boldsymbol{w}}_{\texttt{mle}} = \begin{bmatrix} 1 & -1/\epsilon \\ -1/\epsilon & 2/\epsilon^2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1+\epsilon \\ 1 \end{bmatrix} = \begin{bmatrix} 1+\epsilon \\ -1 \end{bmatrix} = \begin{bmatrix} 1.1 \\ -1 \end{bmatrix}$.
- Maximum a posteriori estimation. Let $\lambda = 0.05$
- $(\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda \boldsymbol{I}_D) = \begin{bmatrix} 2+\lambda & \epsilon \\ \epsilon & \epsilon^2+\lambda \end{bmatrix} = \begin{bmatrix} 2.05 & 0.1 \\ 0.1 & 0.06 \end{bmatrix}$
- $(\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda \boldsymbol{I}_D)^{-1} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix}$
- Ex. 1: $\hat{\boldsymbol{w}}_{\texttt{map}} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.9735 \\ 0.0442 \end{bmatrix}$
- Ex. 2: $\hat{\boldsymbol{w}}_{\texttt{map}} = \begin{bmatrix} 0.531 & -0.885 \\ -0.885 & 18.1416 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1+\epsilon \\ 1 \end{bmatrix} = \begin{bmatrix} 1.0265 \\ -0.0442 \end{bmatrix}$