A Maximum-Likelihood View of Linear Regression

Computer Vision (CSCI 5520G)

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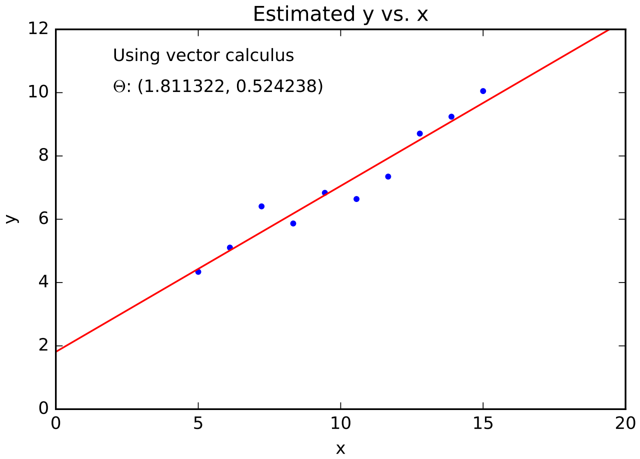
Probabilistic view of linear regression

We now turn our attention to probabilistic view of linear regression.



Univariate Gaussian distribution

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

μ is the center of mass or *mean*

σ^2 is the variance

μ and σ^2 are sufficient statistics

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Sampling from a Gaussian

$$x \sim \mathcal{N}(\mu, \sigma^2)$$

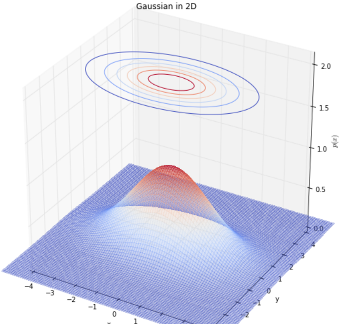
Multivariate Gaussian distribution

Gaussian distribution in d-dimensions

$$\mathcal{N}(\mathbf{x}|\mu, \Sigma) = \frac{1}{|\Sigma|^{\frac{1}{2}}\,(2\pi)^{\frac{d}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1} (\mathbf{x}-\mu)\right)$$

$\mathbf{x}, \mu \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$

Ex: 2D Gaussian



Covariance

Covariance between two random variables X and Y measures the degree to which these variables are linearly related.

$$\mathrm{cov}[X, Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$$

$\mathbb{E}[X]$ is the *expected* value of the random variable X.

$$\mathbb{E}[X] = \int xp(x)dx = \mu$$

Covariance matrix Σ

If $\mathbf{x} \in \mathbb{R}^d$ random vector, its covariance matrix Σ is defined as follows:

$$\Sigma = \mathrm{cov}[\mathbf{x}] = \left[\begin{array}{cccc} \mathrm{var}[X_1] & \mathrm{cov}[X_1, X_2] & \cdots & \mathrm{cov}[X_1, X_d] \\ \mathrm{cov}[X_2, X_1] & \mathrm{var}[X_2] & \cdots & \mathrm{cov}[X_2, X_d] \\ \vdots & \vdots & & \vdots \\ \mathrm{cov}[X_d, X_1] & \mathrm{cov}[X_d, X_2] & \cdots & \mathrm{var}[X_d] \end{array} \right]$$

Likelihood example

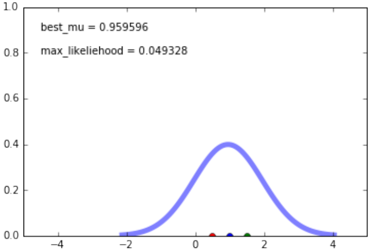
Consider the points: $y_1 = 1$, $y_2 = 0.5$ and $y_3 = 1.5$. The points are drawn from a Gaussian with unknown *mean* θ and $\sigma^2 = 1$.

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

Points are independent so

$$P(y_1, y_2, y_3|\theta) = P(y_1|\theta)P(y_2|\theta)P(y_3|\theta)$$

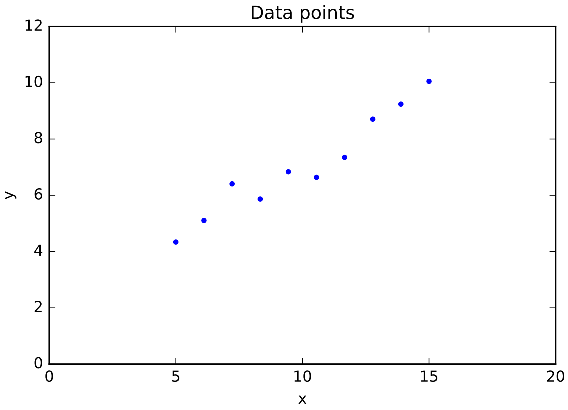
Our goal is to find the Gaussian (i.e., find its mean, since variance is already given) that maximizes the *likelihood* of this data.



From Nando de Freitas

Linear regression

Consider data points $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(N)}, y^{(N)})$. Our goal is to learn a function $f(x)$ that returns (predict) the value y given an x.



Probablistic view of linear regression

Let's assume that targets $y^{(i)}$ are corrupted by Gaussian noise with 0 mean and σ^2 variance

$$
\begin{aligned}
y^{(i)} &= (\theta_0 + \theta_1 x^{(i)}) + \mathcal{N}(0, \sigma^2) \\
&= \mathcal{N}\left(\theta_0 + \theta_1 x^{(i)}, \sigma^2\right)
\end{aligned}
$$

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Why assume Gaussian noise?

- Mathematically convenient
- A reasonably accurate assumption in practice
- Central Limit Theorem

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In higher dimensions

$$y^{(i)} = \mathcal{N}\left(\mathbf{x}^{(i)T}\theta, \sigma^2\right)$$

The likelihood for linear regression

Under the assumption that each $y^{(i)}$ is independant and identically distribtuted (i.i.d.), we can write the likelihood of $\mathbf{y}$ given data $\mathbf{X}$ as follows:

$$
\begin{aligned}
p(\mathbf{y}|\mathbf{X};\theta,\sigma) &= \prod_{i=1}^{N} p(y^{(i)}|\mathbf{x}^{(i)};\theta,\sigma) \\
&= \prod_{i=1}^{n} \left(2\pi\sigma^2\right)^{-1/2} e^{-\frac{1}{2\sigma^2}\left(y^{(i)}-\mathbf{x}^{(i)T}\theta\right)^2} \\
&= \left(2\pi\sigma^2\right)^{-n/2} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y^{(i)}-\mathbf{x}^{(i)T}\theta\right)^2} \\
&= \left(2\pi\sigma^2\right)^{-n/2} e^{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)}
\end{aligned}
$$

Aside: the ";" above indicate that we are following the *frequentist* approach, and we do not treat θ as a random variable. Rather we view θ as having some true value that we are trying to estimate.

Probabilistic view of linear regression

Least squares loss

$$C(\theta) = (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta)$$

Probabilistic view

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Probability of data given parameters is related to the loss for linear regression that we obtained before.

Maximum Likelihood Estimation (MLE)

Likelihood

$$p(\mathbf{y}|\mathbf{X};\theta,\sigma) = \left(2\pi\sigma^2\right)^{-n/2} e^{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)}$$

Negative log-likelihood

$$\begin{aligned} -\log p(\mathbf{y}|\mathbf{X};\theta,\sigma) &= -\log\left(\left(2\pi\sigma^2\right)^{-n/2} e^{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)}\right) \\ &= \frac{n}{2}\log\left(2\pi\sigma^2\right) + \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta) \end{aligned}$$

Maximum likelihood estimation

The maximum likelihood estimate (MLE) of θ is obtained by maximizing $p(\mathbf{y}|\mathbf{X};\theta,\sigma)$

$$\begin{aligned}
\theta_{\mathrm{ML}} &= \arg\max_{\theta}\; p(\mathbf{y}|\mathbf{X};\theta,\sigma) \\
&= \arg\min_{\theta}\; -\log p(\mathbf{y}|\mathbf{X};\theta,\sigma) \\
&= \arg\min_{\theta}\; \frac{n}{2}\log\left(2\pi\sigma^2\right) + \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta) \\
&= \arg\min_{\theta}\; (\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)
\end{aligned}$$

Take away

Maximum likelihood estimate θ_{ML}

$$\theta_{\mathrm{ML}} = \arg\min_{\theta} \underbrace{(\mathbf{y} - \mathbf{X}\theta)^T(\mathbf{y} - \mathbf{X}\theta)}_{\text{MSE Loss}}$$

For model fitting using maximum likelihood estimate, minimize MSE loss.

Making predictions using MLE

For a previously unseen data $\mathbf{x}^*$, the target y^* can be obtained as follows:

$$y^* \sim \mathcal{N}(\theta_{\mathrm{ML}}^T \mathbf{x}^*, \sigma^2)$$

Kullback-Leibler (KL) divergence

Kullback-Leibler divergence is a measure of how much two probability distributions diverge from each other.

$$
\begin{aligned}
D_{\mathrm{KL}}\left(p \| q\right) &= \int p(x) \log \frac{p(x)}{q(x)} dx \\
&= \mathbb{E}_{x \sim p(x)} \left[\log \frac{p(x)}{q(x)} \right]
\end{aligned}
$$

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KL divergence is **not a measure of distance**, since it is not symmetric

$$
D_{\mathrm{KL}}\left(P \| Q\right) \neq D_{\mathrm{KL}}\left(Q \| P\right)
$$

MLE and KL divergence

Consider the setting where we are attempting to fit a distribution $P(x|\theta)$ to data that is drawn from some true distrubtion $P(x|\theta^*)$. One way to do so is to find the parameter θ that minimizes the KL divergence between the two distrubtions.

$$
\begin{aligned}
\theta_{\text{minKL}} &= \arg\min_\theta D_{\text{KL}}\left[P(x|\theta^*) \| P(x|\theta)\right] \\
&= \arg\min_\theta \mathbb{E}_{x\sim P(x|\theta^*)}\left[\log \frac{P(x|\theta^*)}{P(x|\theta)}\right] \\
&= \arg\min_\theta \mathbb{E}_{x\sim P(x|\theta^*)}\left[\underbrace{\log P(x|\theta^*)}_{\text{does not effect minima}} - \log P(x|\theta)\right] \\
&= \arg\min_\theta \mathbb{E}_{x\sim P(x|\theta^*)}\left[-\log P(x|\theta)\right] \\
&= \underbrace{\arg\max_\theta \mathbb{E}_{x\sim P(x|\theta^*)}\left[\log P(x|\theta)\right]}_{MLE}
\end{aligned}
$$

MLE and KL divergence

It turns out that for i.i.d. (independant, identically distributed) data from a some (unknown true) distribution MLE minimizes the KL divergence.

Ridge regression and Bayes rule

Previously we saw the loss function for ridge regression

$$C(\theta) = (\mathbf{y} - \mathbf{X}\theta)^T(\mathbf{y} - \mathbf{X}\theta) + \delta^2\theta^T\theta$$

We can cast the above in probabilistic terms

$$p(y|\mathbf{x}, \theta) = \frac{1}{Z_1} e^{-\left((\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)\right)}$$

Then

$$p(\theta) = \frac{1}{Z_2} e^{-\delta^2\theta^T\theta}$$

becomes *prior*.

Summary

- We developed a probabilistic view of linear regression.
- Maximum likelihood estimation
- Kullback-Leibler divergence
- Relationship between MLE and KL

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