

Probabilistic model of linear regression

Probabilistic model

So far in this course, *a model* referred to a parametric family of functions, such as

$$f(x) = \beta_0 + \beta_1 x.$$

We will now discuss *probabilistic (generative) models*, such as

$$\begin{aligned}y &= \beta_0 + \beta_1 x + \epsilon, \\ \epsilon &\sim \mathcal{N}(0, \sigma^2),\end{aligned}$$

where $\mathcal{N}(0, \sigma^2)$ denotes a Gaussian distribution with mean 0 and variance σ^2 .

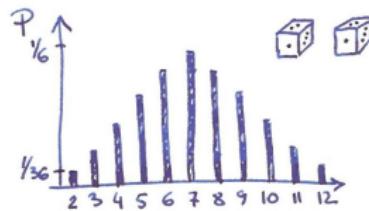
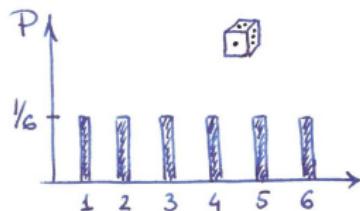


Probability theory recap

Discrete probability distributions

Probability distributions can be *discrete* or *continuous*.

A discrete random variable X is described by a *probability mass function* (PMF):



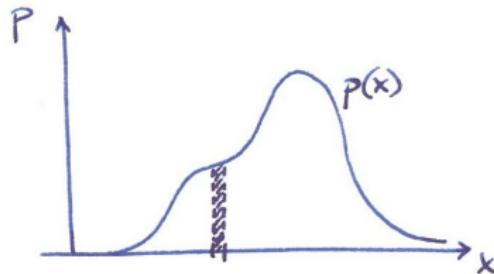
Here X can take values x_i with probabilities p_i , with

$$p_i \geq 0, \quad \sum_i p_i = 1.$$



Continuous probability distributions

A continuous random variable X is described by a *probability density function (PDF)*:



$$p(x) \geq 0,$$

$$\int_{\mathbb{R}} p(x) dx = 1.$$



The mean and the variance

If a discrete random variable X takes values x_i with probabilities p_i , then

$$\mathbb{E}[X] = \sum_i x_i p_i,$$

$$\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \sum_i (x_i - \mathbb{E}[X])^2 p_i.$$

If a continuous random variable X is described by a PDF $p(x)$, then

$$\mathbb{E}[X] = \int x p(x) dx,$$

$$\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \int (x - \mathbb{E}[X])^2 p(x) dx.$$



Variance, covariance, and correlation

We defined

$$\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2].$$

We can similarly define

$$\text{Cov}[X, Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])].$$

Note that

$$\text{Cov}[X, X] = \text{Var}[X].$$

If $\text{Cov}[X, Y] = 0$, then X and Y are *uncorrelated*. Reminder:

$$\text{Corr}[X, Y] = \frac{\text{Cov}[X, Y]}{\sqrt{\text{Var}[X] \text{Var}[Y]}} \in [-1, 1].$$

X and Y are *independent* if their joint distribution factorizes:

$$p_{(X,Y)}(x, y) = p_X(x) \cdot p_Y(y).$$



Some properties of mean and variance

Some useful properties of the expected value:

$$\mathbb{E}[aX] = a\mathbb{E}[X]$$

$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$

$$\mathbb{E}[XY] \neq \mathbb{E}[X]\mathbb{E}[Y] \text{ (unless uncorrelated)}$$

and of variance:

$$\text{Var}[aX] = a^2 \text{Var}[X]$$

$$\text{Var}[X + Y] \neq \text{Var}[X] + \text{Var}[Y] \text{ (unless uncorrelated)}$$

$$\text{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$



Multivariate probability distributions

A random variable X can be *multivariate* (random vector):



$$p(\mathbf{x}) \geq 0,$$

$$\int_{\mathbb{R}^2} p(\mathbf{x}) d\mathbf{x} = 1.$$



Multivariate probability distributions

If a continuous multivariate random variable X is described by a PDF $p(\mathbf{x})$, then

$$\mathbb{E}[X] = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x}.$$

The variance is now replaced by a *covariance matrix*:

$$\text{Cov}[X] = \mathbb{E}\left[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^\top\right].$$

Its diagonal elements are variances of X_i :

$$\text{Cov}[X]_{ii} = \text{Var}[X_i]$$

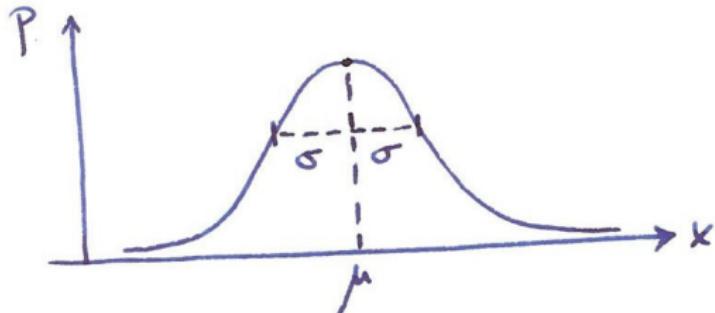
while off-diagonal elements are covariances of X_i and X_j :

$$\text{Cov}[X]_{ij} = \text{Cov}[X_i, X_j].$$



Gaussian distribution

Gaussian (normal) distribution $\mathcal{N}(\mu, \sigma^2)$ with mean μ and variance σ^2 :



$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{(x-\mu)^2}{2\sigma^2} \right]$$

If $\mu = 0$ and $\sigma = 1$, this is called *standard* normal distribution:

$$p(x) = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{x^2}{2} \right].$$



Multivariate Gaussian distribution

Multivariate Gaussian distribution $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ in \mathbb{R}^k with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$:

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k \det(\boldsymbol{\Sigma})}} \exp \left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right].$$

If $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\Sigma} = \mathbf{I}$, this is also called *standard* multivariate normal distribution:

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k}} \exp \left[-\frac{1}{2} \|\mathbf{x}\|^2 \right].$$

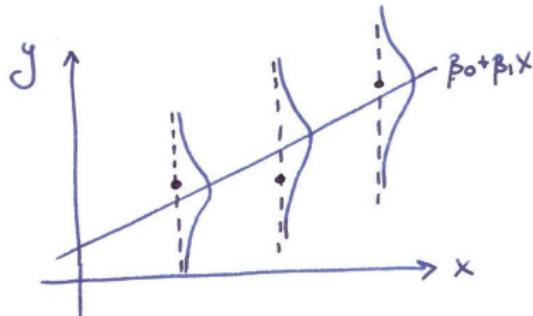


Back to the probabilistic
model for linear regression

Probabilistic model

Probabilistic model for regression:

$$y = \beta_0 + \beta_1 x + \epsilon = \boldsymbol{\beta}^\top \mathbf{x} + \epsilon,$$
$$\epsilon \sim \mathcal{N}(0, \sigma^2).$$



Note: this assumes independent noise (errors) and equal noise variance for all points (*homoscedasticity*).



Likelihood

For a given β and given \mathbf{x}_i ,

$$y^{(i)} \sim \mathcal{N}(\beta^\top \mathbf{x}^{(i)}, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y^{(i)} - \beta^\top \mathbf{x}^{(i)})^2}{2\sigma^2}\right].$$

Probability density to generate the entire training set $\{(\mathbf{x}^{(i)}, y^{(i)})\}$ is

$$\prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y^{(i)} - \beta^\top \mathbf{x}^{(i)})^2}{2\sigma^2}\right].$$

If we re-interpret this as a function of β (and σ^2), then it is called *the likelihood*.



Maximum likelihood

Find β and σ^2 maximizing the likelihood:

$$\prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(y^{(i)} - \beta^\top \mathbf{x}^{(i)})^2}{2\sigma^2}\right].$$

Product of exponentials is annoying to work with \Rightarrow take the logarithm to obtain *log-likelihood*:

$$\begin{aligned} \sum_{i=1}^n & \left[\log\left[\frac{1}{\sigma\sqrt{2\pi}}\right] + \left[-\frac{(y^{(i)} - \beta^\top \mathbf{x}^{(i)})^2}{2\sigma^2}\right] \right] = \\ & = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y^{(i)} - \beta^\top \mathbf{x}^{(i)})^2. \end{aligned}$$

It is often convenient to think about minimizing *the negative log-likelihood*.



Maximum likelihood

Negative log-likelihood:

$$\begin{aligned} \frac{n}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^n (y^{(i)} - \boldsymbol{\beta}^\top \mathbf{x}^{(i)})^2 \\ = \frac{n}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2. \end{aligned}$$

Maximizing likelihood is equivalent for $\boldsymbol{\beta}$ to minimizing squared error!

Exercise: what is the maximum likelihood solution for σ^2 ?



Statistical properties of $\hat{\beta}$

$\hat{\beta}$ is an estimator of β . It is a random variable that depends on the input data. We are interested in the expected value and the (co)variance of this estimator.

We assume \mathbf{X} is fixed and β is fixed. The response vector $\mathbf{y} = \mathbf{X}\beta + \epsilon$ is random. We want to study $\mathbb{E}[\hat{\beta}]$ and $\text{Cov}[\hat{\beta}]$ over ϵ .



$\hat{\beta}$ is an unbiased estimator

Theorem: $\mathbb{E}[\hat{\beta}] = \beta$, i.e. it is an *unbiased* estimator.

Proof:

$$\begin{aligned}\mathbb{E}[\hat{\beta}] &= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}] \\ &= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top (\mathbf{X}\beta + \epsilon)] \\ &= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X}\beta] + \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \epsilon] \\ &= \beta + \mathbf{0} \\ &= \beta.\end{aligned}$$

Note: here we assumed that $n > p$ and \mathbf{X} has *full rank*, i.e. all singular values are non-zero, i.e. $(\mathbf{X}^\top \mathbf{X})^{-1}$ exists.



Covariance matrix of $\hat{\beta}$ and Gauss-Markov

Exercise: $\text{Cov}[\hat{\beta}] = \sigma^2(\mathbf{X}^\top \mathbf{X})^{-1}$.

$\text{Cov}[\hat{\beta}]$ describes uncertainty around $\hat{\beta}$. We see that small singular values of \mathbf{X} lead to large uncertainty.

Gauss-Markov theorem: $\hat{\beta}$ has the smallest variance among all unbiased linear estimators. It is the *best linear unbiased estimator* (BLUE).

What does this mean exactly? That $\text{Var}[\mathbf{a}^\top \hat{\beta}] \leq \text{Var}[\mathbf{a}^\top \tilde{\beta}]$ for any vector \mathbf{a} (or, equivalently, $\text{Cov}[\tilde{\beta}] - \text{Cov}[\hat{\beta}]$ is a *positive semi-definite matrix*, i.e. all singular values are ≥ 0). In particular, $\text{Var}[\hat{\beta}_i] \leq \text{Var}[\tilde{\beta}_i]$ for any i .



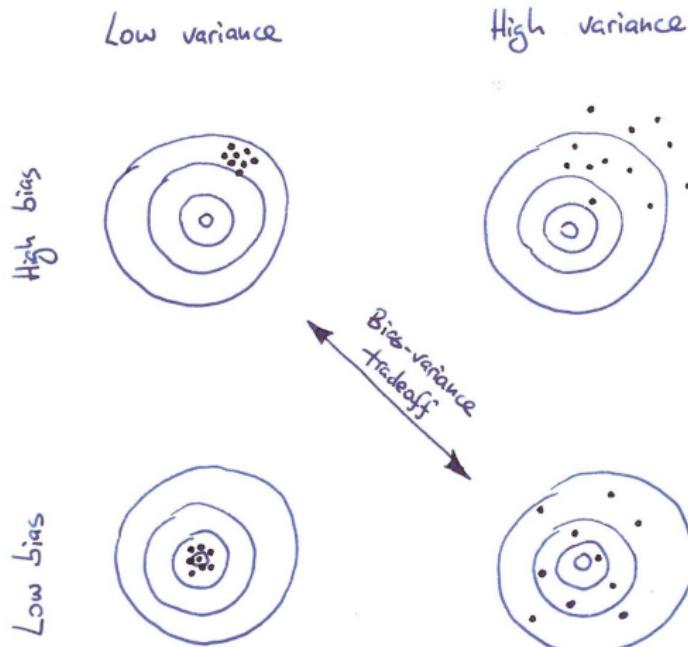
Is the best linear unbiased estimator always the best estimator?

No.



Underfitting, overfitting, and the bias–variance tradeoff

Intuition for bias and variance



Polynomial regression

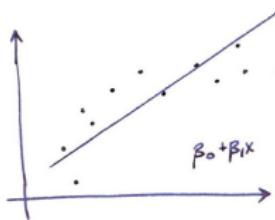
What if we model the relationship between y and x but include x^2, x^3 , etc. terms?

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3.$$

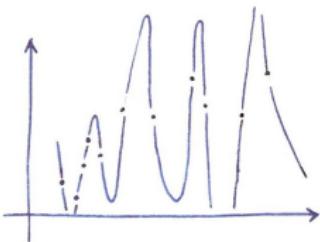
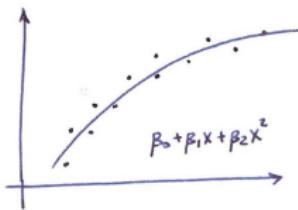
This is *still* linear regression! What?! Yes.



Underfitting and overfitting



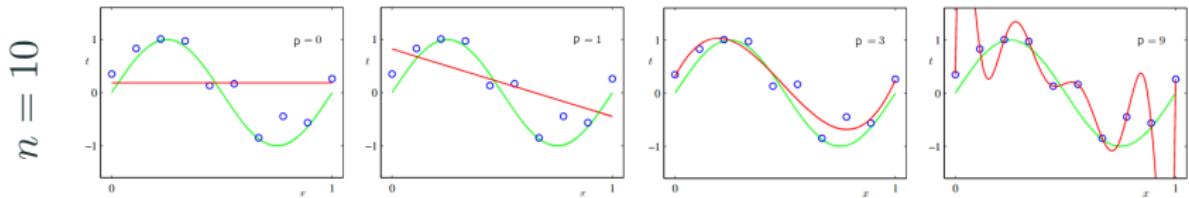
Underfitting
Model too simple
High bias



Overfitting
Model too flexible
High variance



Overfitting and high variance demonstration



	$p = 0$	$p = 1$	$p = 3$	$p = 9$
β_0^*	0.19	0.82	0.31	0.35
β_1^*		-1.27	7.99	232.37
β_2^*			-25.43	-5321.83
β_3^*			17.37	48568.31
β_4^*				-231639.30
β_5^*				640042.26
β_6^*				-1061800.52
β_7^*				1042400.18
β_8^*				-557682.99
β_9^*				125201.43

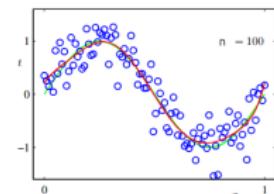
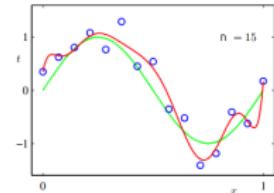


Figure adapted from Bishop, *Pattern Recognition and Machine Learning*



Bias–variance tradeoff

Let $D = \{(x_i, y_i)\}_{i=1}^n$ denote a training dataset, $\hat{f}_D = \hat{f}$ the prediction function, and (x, y) some sample from the data distribution.

$$\begin{aligned}\text{MSE} &= \mathbb{E}_{(x,y);D} \left[(y - \hat{f}(x))^2 \right] \\&= \mathbb{E}_{x,\varepsilon;D} \left[(f(x) + \epsilon - \hat{f}(x))^2 \right] \\&= \mathbb{E}_{x;D} \left[(f(x) - \hat{f}(x))^2 \right] + \sigma^2 \\&= \mathbb{E}_{x;D} \left[(f(x) - \mathbb{E}_D[\hat{f}(x)] + \mathbb{E}_D[\hat{f}(x)] - \hat{f}(x))^2 \right] + \sigma^2 \\&= \mathbb{E}_x \left[(f(x) - \mathbb{E}_D[\hat{f}(x)])^2 \right] + \mathbb{E}_{x;D} \left[(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)])^2 \right] \\&\quad + 2\mathbb{E}_x \left[(f(x) - \mathbb{E}_D[\hat{f}(x)]) \mathbb{E}_D [\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)]] \right] + \sigma^2 \\&= \underbrace{\mathbb{E}_x \left[(f(x) - \mathbb{E}_D[\hat{f}(x)])^2 \right]}_{\text{Bias}^2} + \underbrace{\mathbb{E}_{x;D} \left[(\hat{f}(x) - \mathbb{E}_D[\hat{f}(x)])^2 \right]}_{\text{Variance}} + \sigma^2 \\&= \text{Bias}^2 + \text{Variance} + \sigma^2.\end{aligned}$$



Training and test error

