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

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

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

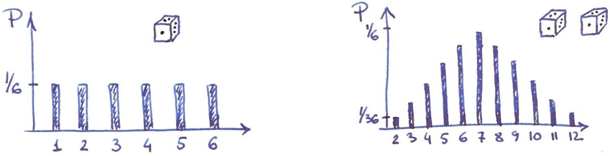
EBERHARD KARLS UNIVERSITÄT TÜBINGEN

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)*:

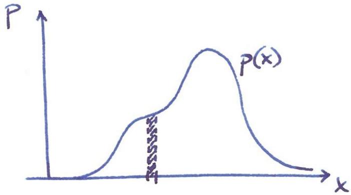


Here X can take values x_i with probabilities p_i, with

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

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

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

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

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

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

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

Variance, covariance, and correlation

We defined
$$\mathrm{Var}[X] = \mathbb{E}\Big[(X - \mathbb{E}[X])^2\Big].$$

We can similarly define

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

Note that
$$\mathrm{Cov}[X, X] = \mathrm{Var}[X].$$

If $\mathrm{Cov}[X, Y] = 0$, then X and Y are *uncorrelated*. Reminder:
$$\mathrm{Corr}[X, Y] = \frac{\mathrm{Cov}[X, Y]}{\sqrt{\mathrm{Var}[X]\,\mathrm{Var}[Y]}}.$$

Some properties of mean and variance

Some useful properties of the expected value:

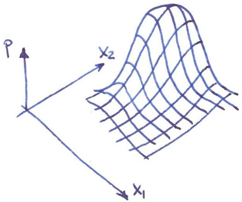
$$\mathbb{E}[aX] = a\mathbb{E}[X]$$
$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$
$$\mathbb{E}[XY] \neq \mathbb{E}[X]\mathbb{E}[Y] \quad \text{(unless independent)}$$

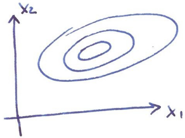
and of variance:

$$\operatorname{Var}[aX] = a^2 \operatorname{Var}[X]$$
$$\operatorname{Var}[X + Y] \neq \operatorname{Var}[X] + \operatorname{Var}[Y] \quad \text{(unless uncorrelated)}$$
$$\operatorname{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$

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*:

$$\mathrm{Cov}[X] = \mathbb{E}\Big[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^\top\Big].$$

Its diagonal elements are variances of X_i:

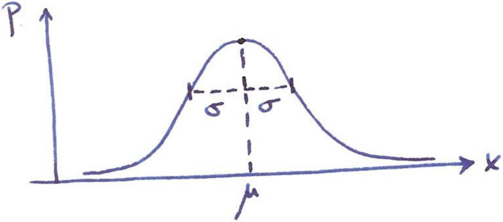
$$\mathrm{Cov}[X]_{ii} = \mathrm{Var}[X_i]$$

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

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

Gaussian distribution

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



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

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

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

Multivariate Gaussian distribution

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

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

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

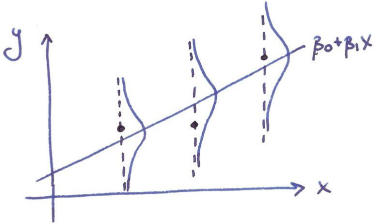
$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k}} \exp\Big[-\frac{1}{2}\|\mathbf{x}\|^2\Big].$$

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 uncorrelated noise (errors) and equal noise variance for all points (*homoscedasticity*).

Likelihood

For a given $\boldsymbol{\beta}$ and given $\mathbf{x}_i$,

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

Probability density to generate the entire training set $\{(\mathbf{x}_i, y_i)\}$ is

$$\prod_i \frac{1}{\sigma\sqrt{2\pi}} \exp\Big[-\frac{(y_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^2}{2\sigma^2}\Big].$$

If we re-interpret this as a function of $\boldsymbol{\beta}$ (and σ^2), then it is called *the likelihood*.

Maximum likelihood

Find β and σ^2 maximizing the likelihood:

$$\prod_i \frac{1}{\sigma\sqrt{2\pi}} \exp\Big[-\frac{(y_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^2}{2\sigma^2}\Big].$$

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

$$\sum_i \Bigg[\log\Big[\frac{1}{\sigma\sqrt{2\pi}}\Big] + \Big[-\frac{(y_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^2}{2\sigma^2}\Big]\Bigg] =$$

$$= -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_i (y_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^2.$$

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

Maximum likelihood

Negative log-likelihood:

$$\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_i (y_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^2 =$$

$$= \frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2.$$

Maximizing likelihood is equivalent 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 $\mathbf{y} = \mathbf{X}\beta + \boldsymbol{\epsilon}$ is random. We want to study $\mathbb{E}[\hat{\beta}]$ and $\mathrm{Cov}[\hat{\beta}]$ over $\boldsymbol{\epsilon}$.

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

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

Proof:

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

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

$\mathrm{Cov}[\hat{\beta}]$ 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 $\mathrm{Var}[\mathbf{a}^\top\hat{\beta}] \le \mathrm{Var}[\mathbf{a}^\top\tilde{\beta}]$ for any vector $\mathbf{a}$ (or, equivalently, $\mathrm{Cov}[\tilde{\beta}] - \mathrm{Cov}[\hat{\beta}]$ is a *positive semi-definite matrix*, i.e. all singular values are ≥ 0).

Is the best linear unbiased estimator always the best estimator?

No.

Underfitting, overfitting, and the bias–variance tradeoff

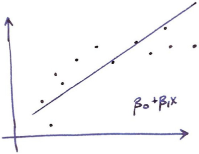
Polynomial regression

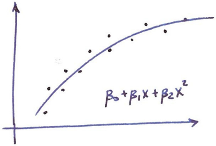
What if we model the relationship between y and x but include x^2, x^3, etc. terms?

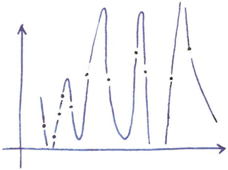
$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3.$$

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

Underfitting and overfitting







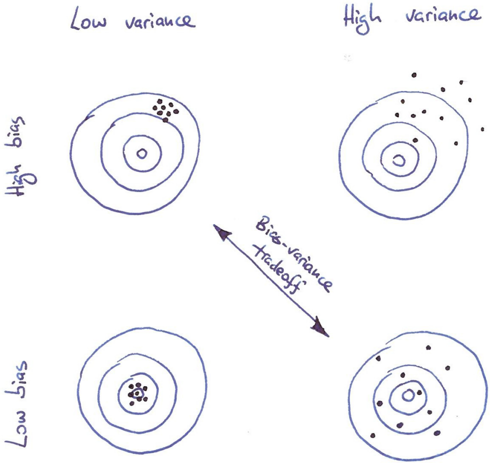
Underfitting
Model too simple
High bias

Overfitting
Model too flexible
High variance

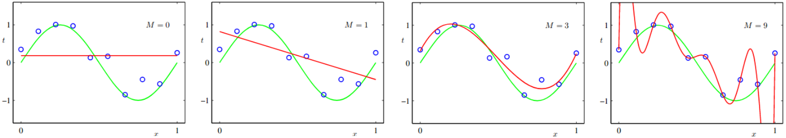
Bias–variance tradeoff

$$
\begin{aligned}
\mathrm{MSE} &= \mathbb{E}\Big[\big(y - \hat f(x)\big)^2\Big] = \\
&= \mathbb{E}\Big[\big(f(x) + \epsilon - \hat f(x)\big)^2\Big] = \\
&= \mathbb{E}\Big[\big(f(x) - \hat f(x)\big)^2\Big] + \sigma^2 = \\
&= \mathbb{E}\Big[\big(f(x) - \mathbb{E}[\hat f(x)] + \mathbb{E}[\hat f(x)] - \hat f(x)\big)^2\Big] + \sigma^2 = \\
&= \Big(f(x) - \mathbb{E}[\hat f(x)]\Big)^2 + \mathbb{E}\Big[\big(\hat f(x) - \mathbb{E}[\hat f(x)]\big)^2\Big] + \\
&\quad + 2\Big(f(x) - \mathbb{E}[\hat f(x)]\Big)\mathbb{E}\Big[\hat f(x) - \mathbb{E}[\hat f(x)]\Big] + \sigma^2 = \\
&= \underbrace{\Big(f(x) - \mathbb{E}[\hat f(x)]\Big)^2}_{\mathrm{Bias}^2} + \underbrace{\mathbb{E}\Big[\big(\hat f(x) - \mathbb{E}[\hat f(x)]\big)^2\Big]}_{\mathrm{Variance}} + \sigma^2 = \\
&= \mathrm{Bias}^2 + \mathrm{Variance} + \sigma^2.
\end{aligned}
$$

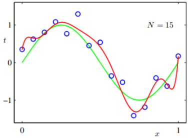
Intuition for bias and variance

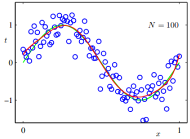


Overfitting and high variance demonstration



	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43





Bishop, *Pattern Recognition and Machine Learning*

Training and test error