# Machine Learning

## Section 8: Linear Regression

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3. November 2021

# Overview

- Regression
- Linear regression
- Maximum likelihood estimation
- Ridge regression
- Bayesian linear regression
- Alternatives

This lecture is based on Chapter 7 of Kevin Murphy's textbook "Machine Learning, A Probabilistic Perspective"

# Regression (1)

## Setup

- data points $(x_1, y_1), \ldots, (x_n, y_n)$
- $x_i$ are locations, usually vectors, sometimes scalars
- $y_i$ are values, usually scalars
- goal: find a function $f$ that maps locations onto values

## Applications / why useful?

- predict celestial orbits (done by 24 year old Gauss, Ceres)
- interpolate measurements (e.g. between climate station)
- smooth noisy measurements (e.g. spectroscopy)
- predict the future (for time locations $x$)

# Regression (2)

## Procedure

- assume a model for function $f$, e.g. for scalar $x$:

$$
\begin{aligned}
f(x) &= w_0 + w_1 x && \text{linear in } x \\
f(x) &= w_0 + w_1 x + w_2 x^2 && \text{nonlinear in } x \\
f(x) &= w_0 + w_1 x + \ldots + w_d x^d && \text{nonlinear in } x
\end{aligned}
$$

- called linear regression since linear in parameter $w$
- fit model with least squares, i.e.

$$w_{\mathrm{LS}} = \arg\min_{w} \sum_{i=1}^{n} (y_i - x_i^T w)^2$$

## Questions

- why least squares? why not absolute values?
- what are the assumptions behind least squares?

# Some of the origins of method of least squares

- C.F. Gauss. *Theoria Motus Corporum Coelestium in Sectionibus Conicis Solem Ambientum*, 1809.
  - method of least squares
  - method of maximum likelihood
  - method of normal distribution
- A.M. Legendre. *Nouvelles méthodes pour la détermination des orbites des comètes*, 1805.

Source:

- `http://en.wikipedia.org/wiki/Regression_analysis#History`
- `http://en.wikipedia.org/wiki/Normal_distribution#Development`

# Notation with many variations

# Linear regression: model specification (1)

## Single data point / linear function

- location $x$ is a vector
- function value at $x$ is modelled as $x^T w$ which is linear in $x$
- *measured* value $y$ is Gaussian distributed around $x^T w$

$$p(y|x, w) = \mathcal{N}(y|x^T w, \sigma^2) \qquad \text{univariate}$$

- $\sigma^2$ is the variance of the measurement noise
- value $y$ is scalar
- parameter $w$ is unknown
- parameter $\sigma^2$ is known
- because $x^T w$ is linear in $w$ this is linear regression

# Linear regression: model specification (2)

## Multiple data points / linear function

- location matrix $X$ contains vectors $x_1, \dots, x_n$ as rows (why rows? see next point)
- function values at $X$ are modelled as $Xw$ which is linear in $X$ (using rows in $X$ makes $Xw$ really simple and minimalistic)
- *measured* values $y$ are Gaussian distributed around $Xw$

$$p(y|X,w) = \mathcal{N}(y|Xw, \Sigma) \qquad \text{multivariate}$$

- vector $y$ contains for each $x_i$ a scalar value
- because $Xw$ is linear in $w$ this is linear regression

# Towards linear regression for nonlinear functions

# Basis function expansion

- for scalar $x$ the polynomial basis function

$$\phi(x) = [1, x, x^2, \ldots, x^d]^T$$

leads to polynomials in $x$

$$\phi(x)^T w = \sum_{i=0}^{d} w_i x^i = w_0 + w_1 x + w_2 x^2 + \ldots + w_d x^d$$

- for vector $x = [x_1, x_2]$ the polynomial basis function

$$\phi(x) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2, \ldots, x_1^d, x_2^d]^T$$

leads to polynomials in $x_1$ and $x_2$ (or simply in $x$):

$$\phi(x)^T w = \sum_{i+j \leq d} w_{ij} x_1^i x_2^j$$

$$= w_{00} + w_{10} x_1 + w_{01} x_2 + w_{20} x_1^2 + w_{02} x_2^2 + w_{11} x_1 x_2 + \ldots + w_{d0} x_1^d + w_{0d} x_2^d$$

- in general $\phi$ maps vector $x$ nonlinearly onto vector $\phi(x)$
- the entries of vector $\phi(x)$ are also called *features*
- $\phi(x)^T w$ is linear in $w$ and possibly nonlinear in $x$

# Linear regression: model specification (3)

Single data point / nonlinear function

- function value at $x$ is modelled as $\phi(x)^T w$ which is nonlinear in $x$
- *measured* value $y$ is Gaussian distributed around $\phi(x)^T w$

$$p(y|x, w) = \mathcal{N}(y|\phi(x)^T w, \sigma^2) \qquad \text{univariate}$$

- because $\phi(x)^T w$ is linear in $w$ this is linear regression

# Linear regression: model specification (4)

## Multiple data points / nonlinear function

- $\phi(X)$ is the matrix with rows $\phi(x_1), \ldots, \phi(x_n)$
- function values are modelled as $\phi(X)w$ which is nonlinear in $X$
- *measured* values $y$ are Gaussian distributed around $\phi(X)w$

$$p(y|X, w) = \mathcal{N}(y|\phi(X)w, \Sigma) \qquad \text{multivariate}$$

- because $\phi(X)w$ is linear in $w$ this is linear regression

## Notes

- $\phi(X)$ has just new locations along the rows
- for readability we consider only $X$ instead of $\phi(X)$
- however, all results hold for both $X$ and $\phi(X)$

Goal: estimate parameter vector $w$

Question

*Why is linear regression called linear?*

Answers:

A Because it is linear in the features.

B Because it is linear in the parameters.

C Because it honors Francois Philippe Marquis de l’Inéar.

D Because it sounds more scientific than just regression.

# Remember:

Linear regression is linear
because it is linear in the parameters.

# Maximum likelihood estimation (1)

## ML estimator

$$\theta_{\mathrm{ML}} = \arg\max_{\theta} p(\mathcal{D}|\theta)$$

- iid data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$
- “iid” means *independent identically distributed*
- iid implies that likelihood factorizes

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{n} p(y_i|x_i, \theta)$$

- this (common) notation is a bit weird, $\mathcal{D}$ was only left of bar, but on RHS $x_i$ is conditioned on
- however, that’s ok, the location is always assumed to be known, also for prediction
- so more precisely, $\mathcal{D}$ only contains the values $y_1, \ldots, y_n$
- better: $p(y|X, \theta) = \ldots$

# Maximum likelihood estimation (2)

Instead to look at the likelihood we consider the

Log-likelihood

$$\begin{aligned}
\ell(w) &= \log p(\mathcal{D}|w) = \sum_{i=1}^{n} \log p(y_i|x_i, w) \\
&= \sum_{i=1}^{n} \log \mathcal{N}(y_i|x_i^T w, \sigma^2) \\
&= -\frac{n}{2\sigma^2} \underbrace{\frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T w)^2}_{\text{mean squared error}} - \frac{n}{2} \log(2\pi\sigma^2)
\end{aligned}$$

- mean squared error (MSE) is also called *sum of squared error*, $\ell_2$ norm of residual errors, etc.
- ML estimation assuming a Gaussian likelihood leads to the method of least squares

# Maximum likelihood estimation (3)

- ML estimation assuming a Gaussian likelihood leads to the method of least squares
- Thus: if we have Gaussian distributed measurements, then least squares is a well-justified method (via ML)
- In Gauss' paper from 1809, he started with the mean which was an established estimator in science (since it is intuitive) and wondered what distribution implies using the mean. By this he invented the normal distriution.

# Maximum likelihood estimation (4)

## Likelihood

$$p(y|X, w) = \mathcal{N}(y|Xw, \Sigma)$$

## Closed-form solution for the ML estimator

$$w_{\text{ML}} = (X^T X)^{-1} X^T y$$

- aka *ordinary least squares* (OLS)
- OLS can be derived by setting the derivative of $\log \mathcal{N}(y|Xw, \Sigma)$ wrt $w$ to zero and solve for $w$

# Maximum likelihood estimation (5)

$d = 1$

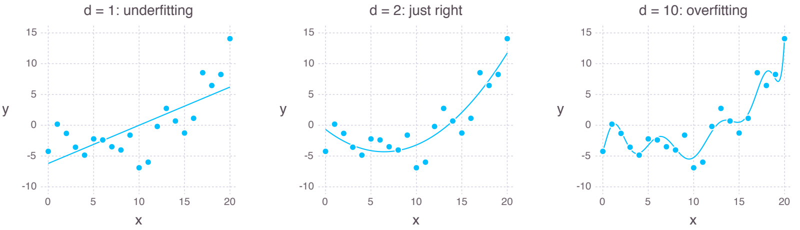
$$f(x) = w_0 + w_1 x$$

$d = 2$

$$f(x) = w_0 + w_1 x + w_2 x^2$$

$d = 10$

$$f(x) = \sum_{i=0}^{10} w_i x^i$$



## Notes

- *underfitting* happens if the model is not flexible enough
- *overfitting* happens if the model is too flexible for the amount of data

# Ridge regression (1)

Overfitting of ML

- too many parameter, too little data
- usually the weights are very large

Idea

- encourage smoother solutions by putting a zero-mean Gaussian prior on *w* to keep it small

$$p(w) = \mathcal{N}(w|0, \tau^2 I)$$

- the variance $\tau^2$ controls the strength of this prior
- do MAP estimation

# Ridge regression (2)

## MAP estimation

$$
\begin{aligned}
w_{\text{ridge}} &= \operatorname{argmax}_w p(w|X,y) = \operatorname{argmax}_w p(y|X,w)p(w|X)/p(y|X) \\
&= \operatorname{argmax}_w p(y|X,w)p(w) \\
&= \operatorname{argmax}_w \sum_{i=1}^{n} \log \mathcal{N}(y_i|x_i^T w, \sigma^2) + \sum_{j=1}^{d} \log \mathcal{N}(w_j|0, \tau^2) \\
&= \operatorname{argmin}_w \underbrace{\frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T w)^2}_{\text{fit}} + \underbrace{\lambda \|w\|_2^2}_{\text{regularizer}}
\end{aligned}
$$

with $\lambda = \sigma^2/\tau^2$ (just move the $\sigma^2$ from the first summand to the second summand and merge with $\tau^{-2}$) and $\|w\|_2^2 = \sum_j w_j^2$.

## Solution

$$
w_{\text{ridge}} = (\lambda I + X^T X)^{-1} X^T y
$$

# Ridge regression (3)

## Solution

$$
\begin{aligned}
w_{\text{ridge}} &= \operatorname{argmin}_w \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda \|w\|_2^2 \\
&= (\lambda I + X^T X)^{-1} X^T y
\end{aligned}
$$

## Notes

- ridge regression is the same as penalized least squares
- $\lambda \|w\|_2^2$ is $\ell_2$ regularization (aka weight decay)

# Ridge regression (4)

Question

- Why regularize by adjusting $\lambda$, why not changing $d$?

Towards an answer

- $d$ sets model complexity
- $\lambda$ measures inverse signal-to-noise ratio (next slides)

# Bayesian linear regression (1)

## Question

- Can we also derive the posterior distribution over $w$ (instead of point estimates via ML and MAP)?

## Prior and likelihood

$$\begin{aligned} p(w) &= \mathcal{N}(w|w_0, V_0) \\ p(y|X, w) &= \mathcal{N}(y|Xw, \Sigma) \end{aligned}$$

## Posterior

$$p(w|X, y) = \mathcal{N}(w|w_n, V_n)$$

$$V_n = (X^T\Sigma^{-1}X + V_0^{-1})^{-1} \qquad \text{posterior covariance}$$

$$w_n = V_n(V_0^{-1}w_0 + X^T\Sigma^{-1}y) \qquad \text{posterior mean}$$

# Bayesian linear regression (2)

## Posterior

$$
\begin{aligned}
p(w|X, y) &= \mathcal{N}(w|w_n, V_n) \\
V_n &= (X^T \Sigma^{-1} X + V_0^{-1})^{-1} && \text{posterior covariance} \\
w_n &= V_n (V_0^{-1} w_0 + X^T \Sigma^{-1} y) && \text{posterior mean}
\end{aligned}
$$

## Notes

- for $\Sigma = \sigma^2 I$, $V_0 = \tau^2 I$, $w_0 = 0$, the mean of the posterior corresponds to ridge regression

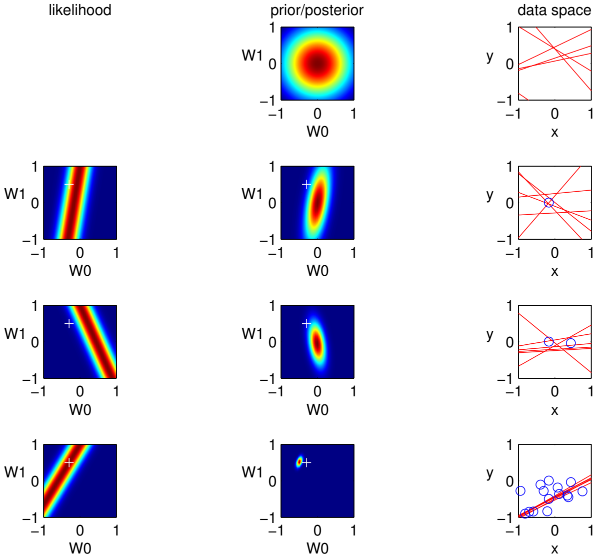
$$w_n = (\lambda I + X^T X)^{-1} X^T y = w_{\text{ridge}}$$

- however, here we have additionally the posterior covariance

$$
\begin{aligned}
V_n &= \sigma^2 (\sigma^2/\tau^2 I + X^T X)^{-1} \\
&= \sigma^2 (\lambda I + X^T X)^{-1}
\end{aligned}
$$

- so $\lambda$ is the inverse signal-to-noise ratio

# Bayesian linear regression (3)



from Murphy's book Figure 7.11

# Bayesian linear regression (4)

## Posterior predictive distribution

- often we want to do prediction
- thus we integrate the parameter out
- training data $\mathcal{D}$ with $n$ pairs of locations and values
- how is value $y$ at a new data location $x$ distributed?

$$\begin{aligned} p(y|x, \mathcal{D}) &= \int \mathcal{N}(y|x^T w, \sigma^2)\, \mathcal{N}(w|w_n, V_n)\, dw \\ &= N(y|x^T w_n, \sigma_n^2) \\ \sigma_n^2 &= \sigma^2 + x^T V_n x \end{aligned}$$

- note that the variance is location dependent
- again for $\Sigma = \sigma^2 I,\ V_0 = \tau^2 I,\ w_0 = 0$:

$$\sigma_n^2 = \sigma^2 (1 + x^T (\lambda I + X^T X)^{-1} x)$$

# Alternatives to least squares (1)

Linear regression

$$p(y|x,w) = \mathcal{N}(y|x^T w, \Sigma)$$

Robust linear regression

$$p(y|x,w) = \mathrm{Lap}(y|x^T w, b) = \exp(-\frac{1}{b}\|y - x^T w\|)/Z(b)$$

# Alternatives to least squares (2)

## Likelihoods and priors for linear regression

| Likelihood | Prior | Name |
|---|---|---|
| Gaussian | Uniform | Least squares |
| Gaussian | Gaussian | Ridge regression |
| Gaussian | Laplace | Lasso |
| Laplace | Uniform | Robust regression |
| Student | Uniform | Robust regression |

copied from Murphy's book Table 7.1

- note that, uniform prior leads to ML
- however, such a uniform prior can often not be normalized

# End of Section 08