Applied Probabilistic Machine Learning

Linear, Kernel, and logistic Regression

Hugues Richard *RichardH@rki.de*
Ivan Tunov *Ivan.Tunov@student.hpi.uni-potsdam.de*

MF1 - Genome Competence Center Robert Koch Institute (RKI)
DACS Hasso Plattner Institute (HPI)

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Reminder - Supervised Learning

Training data $\mathcal{D} = (\mathbf{x}_i, y_i)_{i=1,\dots,n}$

Find a function $\hat{f} : \mathbf{x} \to \hat{f}(\mathbf{x}) = \mathbf{y}$

Classification

$$\mathbf{y} \in \mathcal{C} = \{0, 1\} \text{ (binary)}$$
$$= \{1, \dots, C\} \text{ (multiclass)}$$

Min. misclassification error:

$$\arg\min_{\hat{f}} \sum_{i=1}^{n} |\hat{f}(x_i) - y_i|$$

$$\left(\sum_{i=1}^{n} |\hat{f}(x_i) - y_i| = \sum_i \mathbb{I}_{\{\hat{f}(x_i) \neq y_i\}}\right)$$

Regression

$$\mathbf{y} \in \mathbb{R}$$

Minimize a loss function ℓ

$$\sum_{i=1}^{n} \ell(\hat{f}(x_i) - y_i)$$

(*e.g.* $\ell(x) = x^2, \ell(x) = |x|, \dots$)

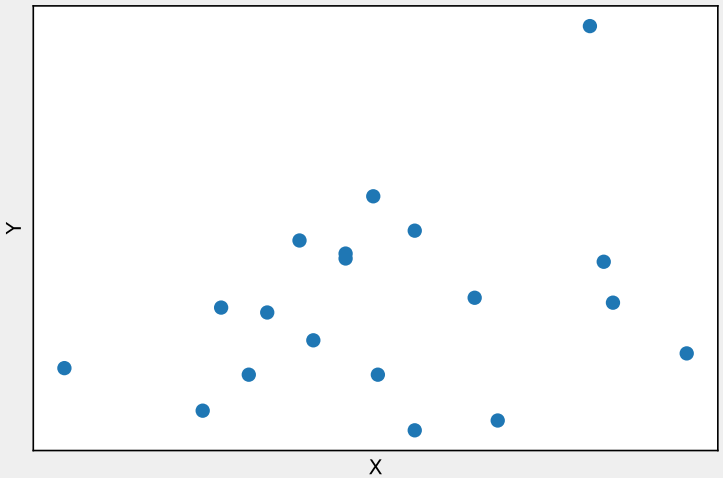
Learning goals

- Understand linear regression and the probabilistic foundation between regression models
- Understand kernel regression when the relationship between features and outcome is not linear
- Understand logistic regression for classification.

Linear Regression

Linear Regression

Let $\mathbf{Y}$ be the dependent variable (response variable) and $\mathbf{X}$ the independent variable (covariate, or predictor):



We assume the following model

$$\mathbf{Y} = f(\mathbf{X}) + \epsilon$$

where f is a linear function that models the expectation $\mathbb{E}[\,Y \,|\, X]$, and ϵ is a noise term (e.g. $\epsilon \sim \mathrm{Normal}(0, \sigma^2)$)

Linear Regression

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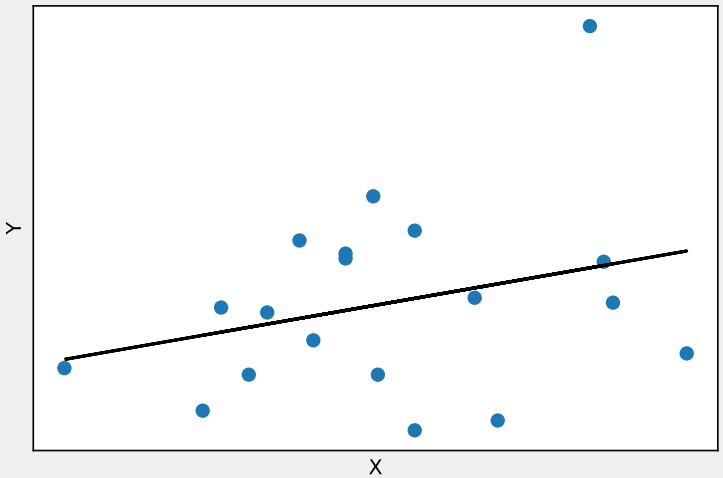

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Linear Regression

- We can also write $\mathbf{Y} \sim \mathrm{Normal}(f(\mathbf{X}), \sigma^2)$
- We assume no distribution for $\mathbf{X}$
- We assume f is a linear function, i.e.

$$f(x) = ax + b$$

- How can we generate data $(x_i, y_i)_i$ with this model?
  - For $i = 1, \ldots, n$:
    - Select some value for x_i
    - Draw ϵ_i from $\mathrm{Normal}(0, \sigma^2)$
    - Compute $y_i = f(x_i) + \epsilon_i$

Linear Regression - Parameter estimation

- In the Bayesian framework, parameters are estimated using the posterior distribution

- We want to know the probability of our hypothesis or parameters $\theta = (a, b)$ given a set of n observations $x = (x_i)_{i=1}^n$ and $y = (x_i)_{i=1}^n$

- An estimate $\hat{\theta}$ of our parameters θ can be computed as the *maximum a posterior (MAP) estimate*

$$\hat{\theta} = \arg\max_{\theta} \ \mathbb{P}(\theta \,|\, x, y)$$

- There are other choices, for instance the *posterior expectation*, which all have their justifications

- We use the MAP for linear regression, because it leads to a computationally simple solution

Linear Regression - Parameter estimation

- For a flat prior, the MAP is equivalent to the *maximum likelihood estimate (MLE)*, i.e.

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} \ \mathbb{P}(\theta \,|\, x, y) \\ &= \arg\max_{\theta} \ \frac{\mathbb{P}(x, y \,|\, \theta)\mathbb{P}(\theta)}{\mathbb{P}(x, y)} \\ &= \arg\max_{\theta} \ \mathbb{P}(x, y \,|\, \theta)\mathbb{P}(\theta) \\ &= \arg\max_{\theta} \ \mathbb{P}(x, y \,|\, \theta)\end{aligned}$$

  assuming $\mathbb{P}(\theta)$ is constant[1]

- This result is not specific to linear regression models

[1] A uniform prior $\mathbb{P}(\theta)$ is called *improper prior* when θ is a continuous variable, because $\mathbb{P}(\theta)$ does not integrate to one

Linear Regression - Parameter estimation

- Furthermore, we have

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} \ \mathbb{P}(x, y \,|\, \theta) \\ &= \arg\max_{\theta} \ \mathbb{P}(y \,|\, x, \theta)\mathbb{P}(x \,|\, \theta) \\ &= \arg\max_{\theta} \ \mathbb{P}(y \,|\, x, \theta)\end{aligned}$$

- In the last step we took advantage of the fact that the distribution of our covariates x does not depend on the parameters θ, which are the slope and intercept of the linear function

- In fact, we do not have do assume a particular distribution for our covariates!

Linear Regression - OLS

- Plugging in our normal distribution we arrive at

$$
\begin{aligned}
\hat{\theta} &= \arg\max_{\theta} \mathbb{P}(y_1 \dots y_n \mid x_1, \dots, x_n, \theta) \\
&= \arg\max_{\theta} \prod_{i=1}^{n} \mathbb{P}(y_i \mid x_i, \theta) \\
&= \arg\max_{\theta} \sum_{i=1}^{n} \log \mathbb{P}(y_i \mid x_i, \theta) \\
&= \arg\max_{\theta} \sum_{i=1}^{n} \log \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{ -\frac{(y_i - f(x_i))^2}{2\sigma^2} \right\} \\
&= \arg\max_{\theta} \sum_{i=1}^{n} -(y_i - f(x_i))^2
\end{aligned}
$$

Linear Regression - OLS

- The estimate

$$\hat{\theta} = \arg\min_{\theta} \sum_{i=1}^{n} (y_i - f(x_i))^2$$
$$= \arg\min_{\theta} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

  is called the *ordinary least squares (OLS)* estimate

- It minimizes the squared error between our prediction $\hat{y}_i$ and our observations y_i

- In other words, it minimizes the squared residuals $\epsilon_i = y_i - f(x_i)$

Linear Regression - Generalization

- For generalizing linear regression to multiple predictors, we first define

$$x = \begin{bmatrix} 1 \\ \tilde{x} \end{bmatrix}, \qquad \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

  i.e. x is a vector where the first component is always 1

- This definition allows to write

$$\begin{aligned} f(x) &= b + a\tilde{x} \\ &= \theta_1 + \theta_2 \tilde{x} \\ &= \begin{bmatrix} 1 \\ \tilde{x} \end{bmatrix}^\top \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \\ &= x^\top \theta \end{aligned}$$

Linear Regression - Generalization

- Adding additional predictors is now very simple

$$x = \begin{bmatrix} 1 \\ x^{(2)} \\ \vdots \\ x^{(p)} \end{bmatrix}, \qquad \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix}$$

- The number of predictors / features is given by p, where the first predictor is $(1, 1, \ldots, 1)^\top$

- It follows that

$$\begin{aligned} f(x) &= x^\top \theta \\ &= \theta_1 + x^{(2)}\theta_2 + \cdots + x^{(p)}\theta_p \end{aligned}$$

Linear Regression - Notation

- In general, we have n observations and p predictors
- For the ith observation (x_i, y_i), y_i is a scalar and x_i a vector

$$x_i = (1, x_i^{(2)}, \dots, x_i^{(p)})^\top$$

- We define the matrix

$$X = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(p)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(p)} \\ \vdots & \vdots & \ddots & \vdots \\ x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(p)} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(2)} & \dots & x_1^{(p)} \\ 1 & x_2^{(2)} & \dots & x_2^{(p)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n^{(2)} & \dots & x_n^{(p)} \end{bmatrix}$$

Linear Regression - Notation

- This notation allows us to write linear regression as

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(2)} & \dots & x_1^{(p)} \\ 1 & x_2^{(2)} & \dots & x_2^{(p)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n^{(2)} & \dots & x_n^{(p)} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

- Or in matrix notation simply as

$$y = X\theta + \epsilon$$

Data matrix X

For a data matrix $X \in \mathbb{R}^{n \times p}$, rows will always correspond to observations and columns correspond to features. The first column is the vector $(1, 1, \dots, 1)^\top$. We always assume that X has full rank, i.e. $\mathrm{rank}(X) = \min(n, p)$

Linear Regression - OLS

If $n > p$ and $X^\top X$ has full rank we can use ordinary least squared (OLS) to estimate θ:

$$\hat{\theta} = \arg\min_{\theta} \|\epsilon\|_2^2 = \arg\min_{\theta} \|y - X\theta\|_2^2$$

Differentiation with respect to θ and solving for the roots leads to:

$$\begin{aligned} \Rightarrow \qquad \hat{\theta} &= (X^\top X)^{-1} X^\top y \\ &= X^\top y \qquad\qquad \text{if } X^\top X = I \end{aligned}$$

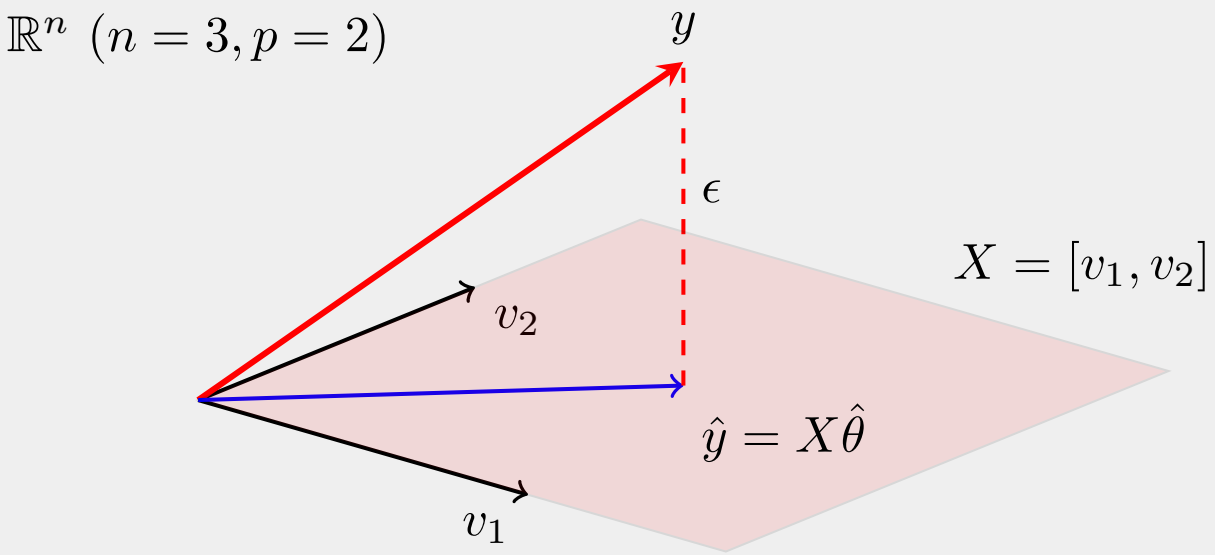
$X(X^\top X)^{-1} X^\top$ is called a projection matrix...

see exercise sheet for the derivation of the solution

Linear Regression - OLS Projection

Let $X\theta = v_1\theta_1 + v_2\theta_2 + \ldots v_p\theta_p$, where v_i denotes the ith column of X

$$\hat{\theta} = \arg\min_{\theta} \|y - X\theta\|_2^2$$



$X(X^\top X)^{-1}X^\top y$ projects y onto the plane defined by the columns of X

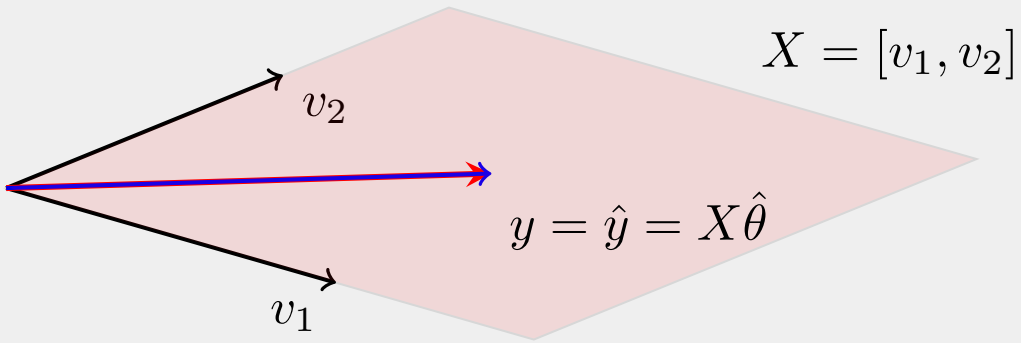
[1] [Hastie et al., 2009, Bishop, 2006]

Linear Regression - OLS Projection

Let $X\theta = v_1\theta_1 + v_2\theta_2 + \ldots v_p\theta_p$, where v_i denotes the ith column of X

$$\hat{\theta} = \arg\min_{\theta} \|y - X\theta\|_2^2$$

$\mathbb{R}^n$ $(n = 3, p = 2)$



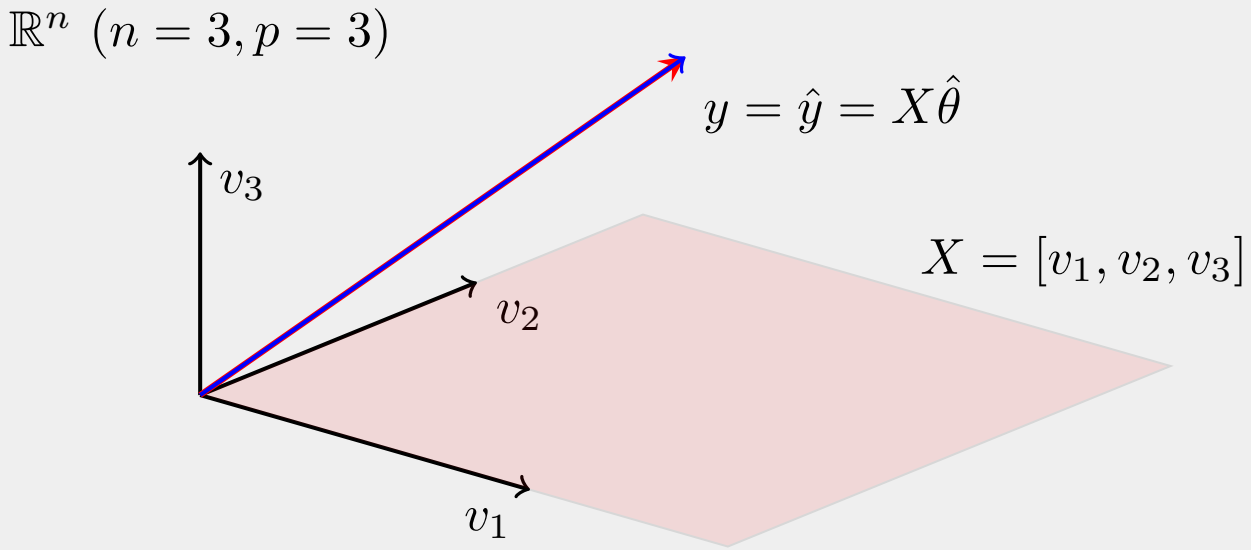
If y is already inside the plane, we obtain $\epsilon = 0$

[1] [Hastie et al., 2009, Bishop, 2006]

Linear Regression - OLS Projection

Let $X\theta = v_1\theta_1 + v_2\theta_2 + \ldots v_p\theta_p$, where v_i denotes the ith column of X

$$\hat{\theta} = \arg\min_{\theta} \|y - X\theta\|_2^2$$



If $p \geq n$ then $\epsilon = 0$ and for $p > n$ we have infinitely many solutions (assuming v_i are pairwise independent)

[1] [Hastie et al., 2009, Bishop, 2006]

Linear Regression - Underdetermined OLS

- For $p > n$ the OLS estimate

$$\hat{\theta} = \arg\min_{\theta} \|y - X\theta\|_2^2$$

has infinitely many solution $\hat{\theta}$ such that $\left\|y - X\hat{\theta}\right\|_2^2 = 0$!

Linear Regression - Underdetermined OLS

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- Which one should we choose?

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- Which one should we choose?

- Remember our initial model

$$y = X\theta + \epsilon$$

and yet the estimate $\hat{\theta}$ satisfies $y = X\hat{\theta}$

Linear Regression - Underdetermined OLS

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- Which one should we choose?
- Remember our initial model

$$y = X\theta + \epsilon$$

and yet the estimate $\hat{\theta}$ satisfies $y = X\hat{\theta}$

- Either $\epsilon = 0$ or $\hat{\theta}$ contains all the noise

Linear Regression - Underdetermined OLS

For instance, we could take that θ with minimal length, i.e. the minimum ℓ_2-norm solution[2]

$$\arg\min_{\theta} \ \|\theta\|_2^2$$
$$\text{subject to } X\theta = y$$

The solution is almost equivalent to the standard OLS solution, i.e.

$$\hat{\theta} = (X^\top X)^+ X^\top y$$

where $(X^\top X)^+$ Moore-Penrose pseudoinverse[3] of $X^\top X$.

[2] Common practice for training neural networks

[3] The Moore-Penrose pseudoinverse of a matrix X is computed as follows: Let $X = S\Sigma V^\top$ be the singular value decomposition of X, where Σ is a diagonal matrix containing the singular values. $X^+ = S\Sigma^+ V^\top$ where Σ^+ contains the reciprocal of all non-zero singular values.

Ridge Regression

The ridge regression estimate is defined as

$$\hat{\theta}(\lambda) = \arg\min_{\theta} \ \|X\theta - y\|_2^2 + \lambda \|\theta\|_2^2$$

where λ is called the *regularization strength* or *penalty*. Note that $\|\theta\|_2^2 = \sum_{i=2}^{n} \theta_i^2$, i.e. θ_1 is not constrained

- There exists an analytical solution to the ridge estimate:

$$\hat{\theta}(\lambda) = (X^\top X + \lambda I)^{-1} X^\top y$$

- In the overparameterized case, for $\lambda > 0$ we obtain $\|\epsilon\|_2^2 > 0$

[3] Convex optimization: [Boyd and Vandenberghe, 2004]

Linear Regression - Ridge Regression

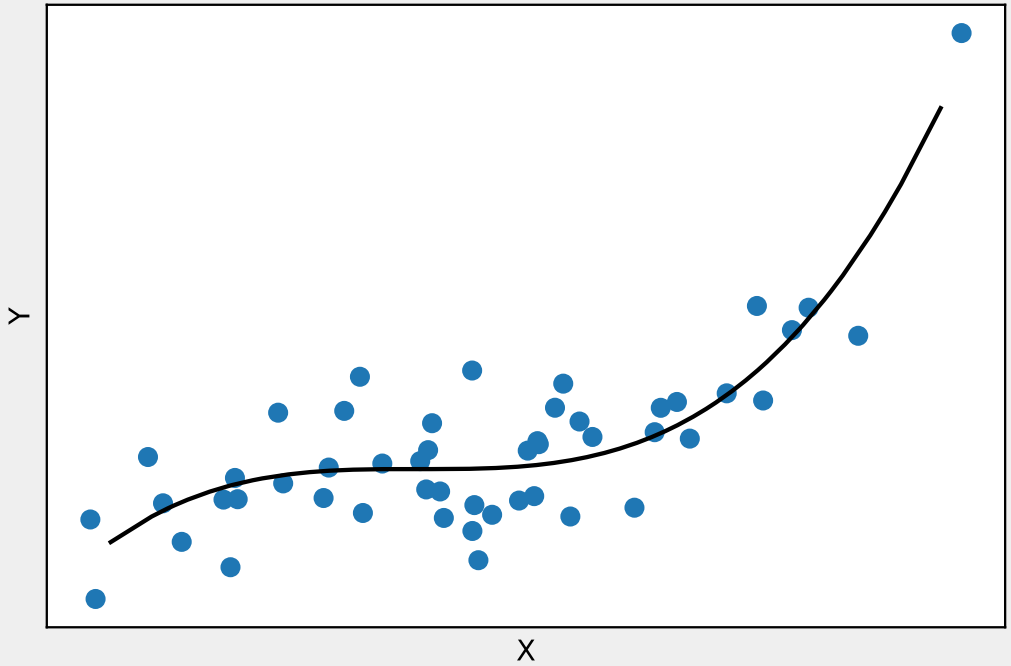
- For $\lambda \to \infty$ the estimate $\lambda\hat{\theta}(\lambda)$ converges to the componentwise regression estimator
- For $\lambda \to 0$ the estimate $\hat{\theta}(\lambda)$ converges to the minimum ℓ_2-norm OLS solution[4]
- The penalty $\lambda \|\theta\|_2^2$ can be interpreted as a Gaussian prior
- Ridge regression is useful when $n < p$ and $n \geq p$

[4] $A + \lambda I$ is invertible even for very small λ. In numerics, $A + \lambda I$ is also used as a trick to ensure that a matrix is positive-definite.

Kernel Regression

Polynomial Regression

- How can we change linear regression to model non-linear relations between $\mathbf{X}$ and $\mathbf{Y}$?



Regression in Feature Space

Polynomial regression

$$\mathbf{Y} = \theta_1 + \theta_2 \mathbf{X} + \theta_3 \mathbf{X}^2 + \theta_4 \mathbf{X}^3 + \cdots + \epsilon\,,$$

More generally, we write

$$\mathbf{Y} = \phi(\mathbf{X})\theta + \epsilon\,,$$

where $\phi : \mathbb{R}^p \to \mathbb{R}^{p'}$ is a feature map that maps points in p-dimensional input space into a p'-dimensional feature space, e.g.

$$\phi(\mathbf{X}) = (1, \mathbf{X}, \mathbf{X}^2, \mathbf{X}^3, \dots)$$

Basically linear (or ridge) regression in p'-dimensional feature space, but non-linear in input space

Kernel Regression

- What if we do not know the exact set of features for our data?
- Can we simply test a large amount of possible features?
- Can we have more features than observations, i.e. $n \leq p$?

Ridge regression in feature space:

$$\hat{\theta}(\lambda) = \arg\min_{\theta} \; \|\phi(X)\theta - y\|_2^2 + \lambda \|\theta\|_2^2$$

where ϕ is applied to each row of X, i.e. $\phi(X) \in \mathbb{R}^{n \times p'}$.

Computationally expensive if $p' \gg p$ and $n \gg 1$, assuming X is not sparse.

Kernel Regression

Reformulate the ridge regression estimate

$$\hat{\theta}(\lambda) = \arg\min_{\theta} \ \|\phi(X)\theta - y\|_2^2 + \lambda \|\theta\|_2^2$$

using kernels. Let $\theta = \phi(X)^\top \eta$, where $\eta \in \mathbb{R}^n$ is a new parameter vector and $\theta \in \text{span}(\phi(x_1), \ldots, \phi(x_n)) \subset \mathbb{R}^p$. It follows that

$$\begin{aligned}\hat{\eta}(\lambda) &= \arg\min_{\eta} \ \left\|\phi(X)\phi(X)^\top \eta - y\right\|_2^2 + \lambda \left\|\phi(X)^\top \eta\right\|_2^2 \\ &= \arg\min_{\eta} \ \|K\eta - y\|_2^2 + \lambda \eta^\top K \eta\end{aligned}$$

where $K = \phi(X)\phi(X)^\top \in \mathbb{R}^{n \times n}$ is the kernel matrix.

Definition: Kernel function

A function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *kernel* if there exists a feature map $\phi : \mathcal{X} \to \mathcal{F}$ such that

$$\kappa(x_i, x_j) = \phi(x_i)^\top \phi(x_j)$$

$K = (\kappa(x_i, x_j))_{x_i \in \mathcal{X}, x_j \in \mathcal{X}}$ is called the kernel matrix.

- $\mathcal{X}$ can be an arbitrary space, for instance DNA sequences
- $\kappa(x_i, x_j)$ is interpreted as a similarity measure in feature space
- Evaluating $\kappa(x_i, x_j)$ does not always require to explicitly compute $\phi(x)$
- Not having to map data into feature space is called the kernel trick

Example Kernels

- Linear kernel

$$\kappa(x_i, x_j) = x_i^\top x_j, \text{ where } \phi(x) = x$$

- Polynomial kernel

$$\kappa(x_i, x_j) = (x_i^\top x_j + 1)^d$$

where $d > 0$ is the degree. For $\mathcal{X} = \mathbb{R}^2$ and $d = 2$

$$\phi(x) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)^\top$$

- Radial basis function (RBF) kernel

$$\kappa(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|_2^2}{2\sigma^2}\right)$$

where the feature space has infinite dimensions

Predictions

Let x_{new} denote the position where we would like to compute a prediction $\hat{y}$

- Linear Regression

$$\hat{y} = \phi(x_{\text{new}})^\top \hat{\theta}$$

- Kernel Regression

$$\hat{y} = \sum_{i=1}^{n} \kappa(x_i, x_{\text{new}}) \hat{\eta}_i = \phi(x_{\text{new}})^\top \phi(X)^\top \hat{\eta}$$

  which requires the full training set $X = (x_i)_i \in \mathbb{R}^{n \times p}$, where we simply used the definition $\theta = \phi(X)^\top \eta$ to replace $\hat{\theta}$ in the prediction of the linear regression model

Parameters and Hyperparameters

- We call θ and η the parameters of a (kernel) regression model
- The parameters of a kernel function (e.g. σ^2 for the RBF kernel) or the regularization strength λ are also parameters of the model, but one step further up the hierarchy
- We call the parameters of a kernel function and the regularization strength hyperparameters
- In a Bayesian setting, the parameters control the likelihood function, whereas the hyperparameters parametrize the prior distribution

Kernel Regression - Pros and Cons

Pros:

- Computationally efficient regression for high-dimensional feature spaces for moderate data sets
- Implicit regularization, i.e. only as many parameters as data points (but equivalent to minimum ℓ_2-norm solution of standard regression)

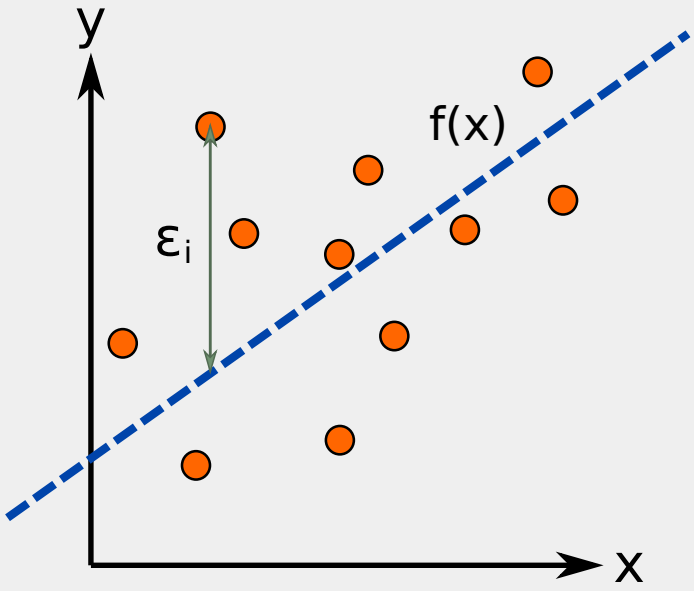
Cons:

- Kernel matrix grows quadratically with number of samples
- $\theta \in \mathbb{R}^p \rightsquigarrow \eta \in \mathbb{R}^n$, which creates dependencies between features
- Interpretation of parameters in feature space requires computation of $\phi(X)^\top \eta$
- For infinite feature spaces ϕ cannot be computed
- No feature selection possible (ℓ_1 penalty)

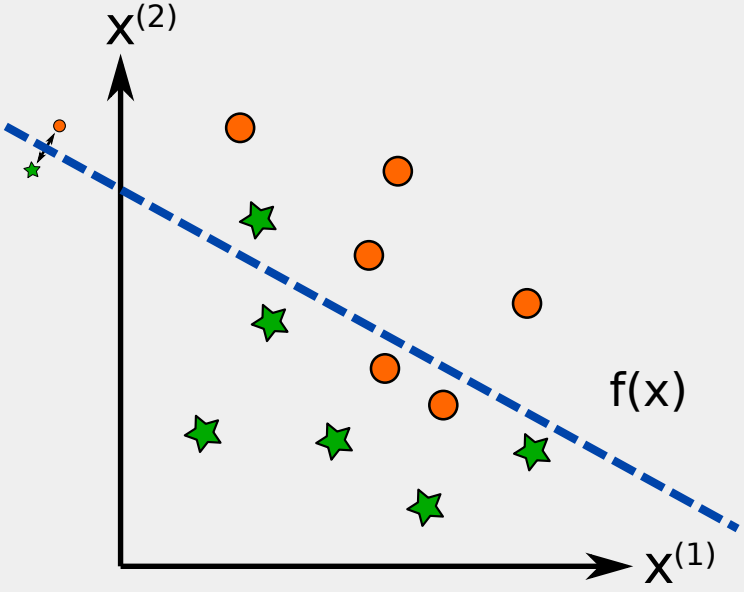
Logistic Regression (Classification)

Linear regression and classification

Linear regression



Logistic regression



$$y = X\theta + \epsilon\,, \quad y \in \mathbb{R} \qquad y \stackrel{?}{=} \sigma(X\theta) + \epsilon\,, \quad y \in \{0, 1\}$$

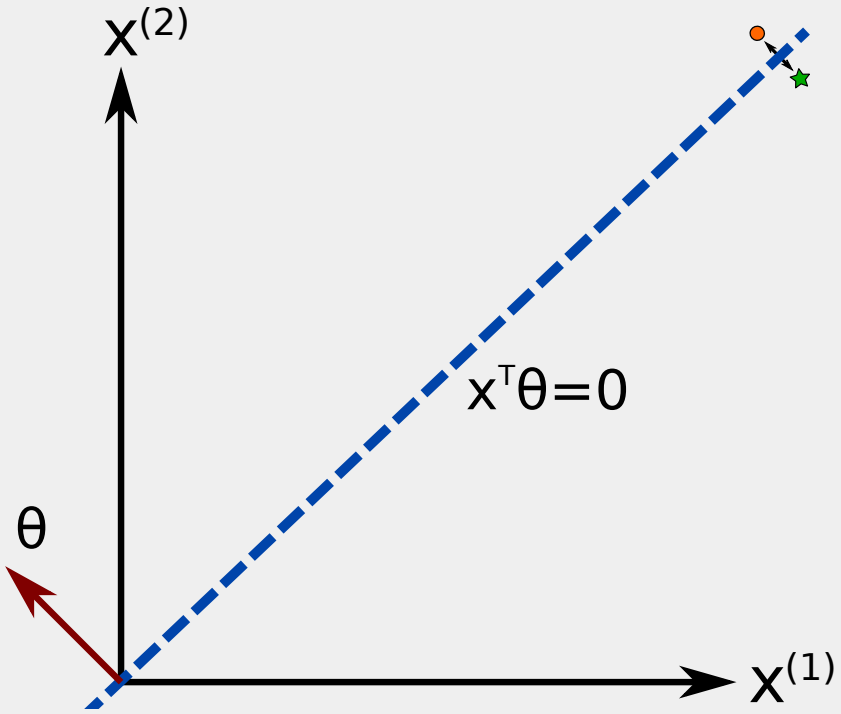
How is the hyperplane defined? What is σ?

Defining hyperplanes

- We use the properties of the dot product to define the separating hyperplane:

$$x^\top \theta = \|x\| \, \|\theta\| \cos \measuredangle$$

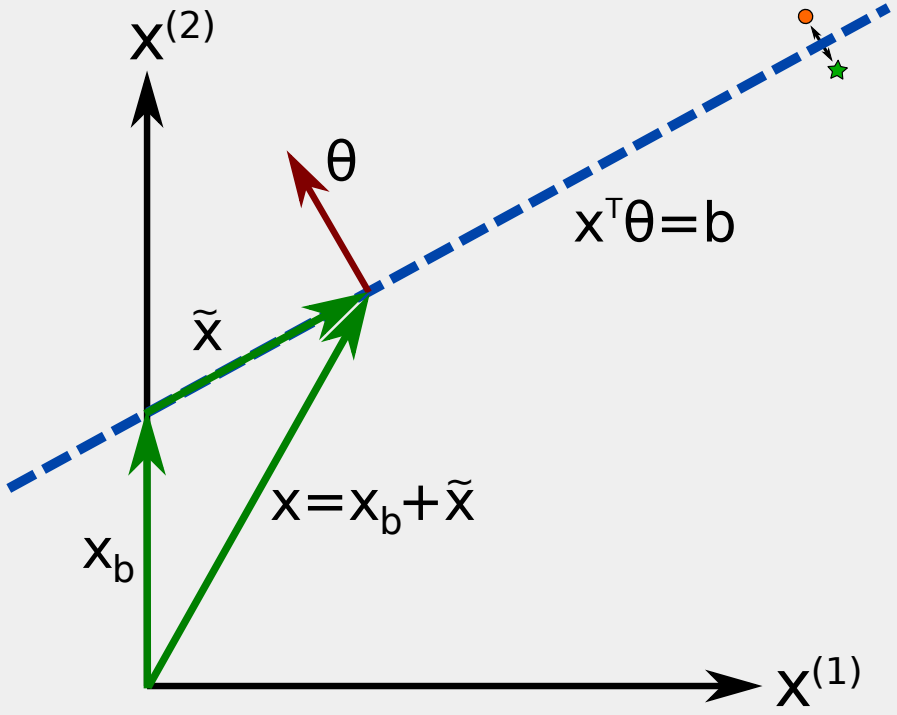
- For vectors x perpendicular to θ we have $\cos \measuredangle = 0$



Defining hyperplanes

- For hyperplanes with bias b we use $x^\top \theta = b$

$$
\begin{aligned}
x^\top \theta &= (x_b + \tilde{x})^\top \theta \\
&= \underbrace{x_b^\top \theta}_{=b} + \underbrace{\tilde{x}^\top \theta}_{=0}
\end{aligned}
$$



Defining hyperplanes

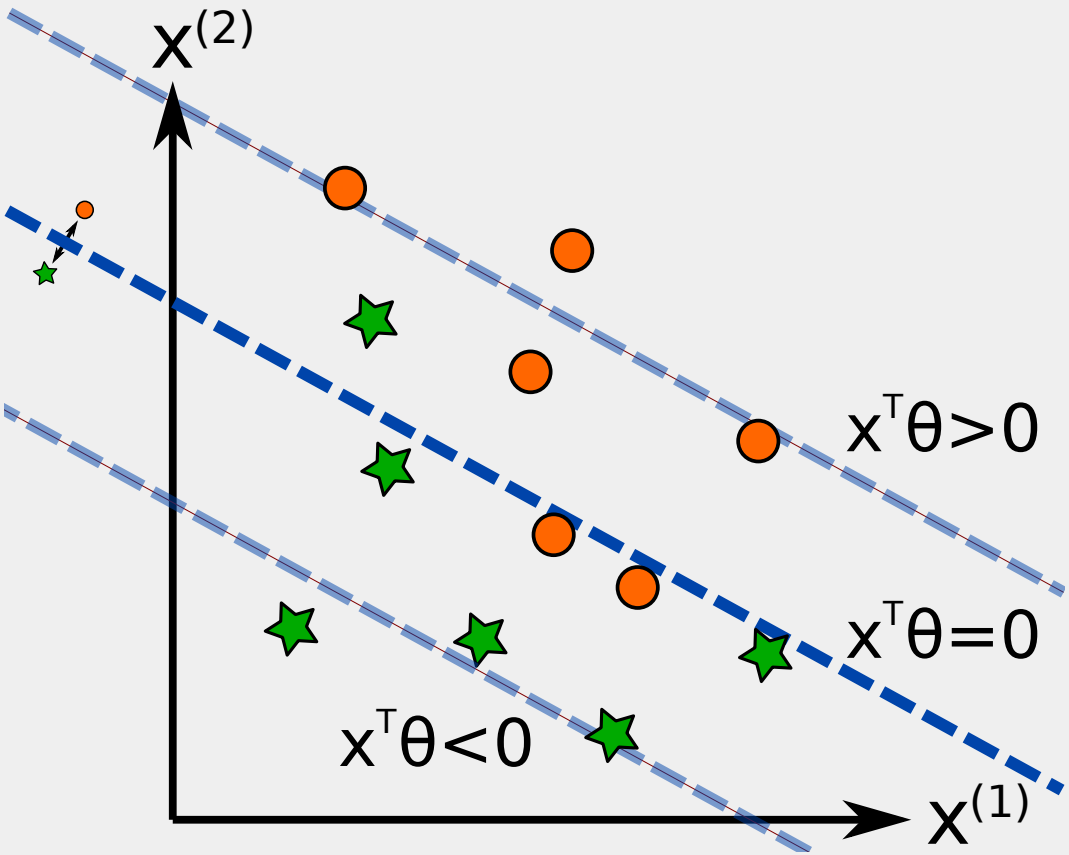
- Remember our convention:

$$x = \begin{bmatrix} 1 \\ x^{(2)} \\ \vdots \\ x^{(p)} \end{bmatrix}, \qquad \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix}$$

- Hence, instead of $x^\top \theta = b$ we can write $x^\top \theta = 0$, because $\theta_1 = -b$

Separating hyperplane

- $x^\top \theta > 0$: predicting positive class
- $x^\top \theta < 0$: predicting negative class



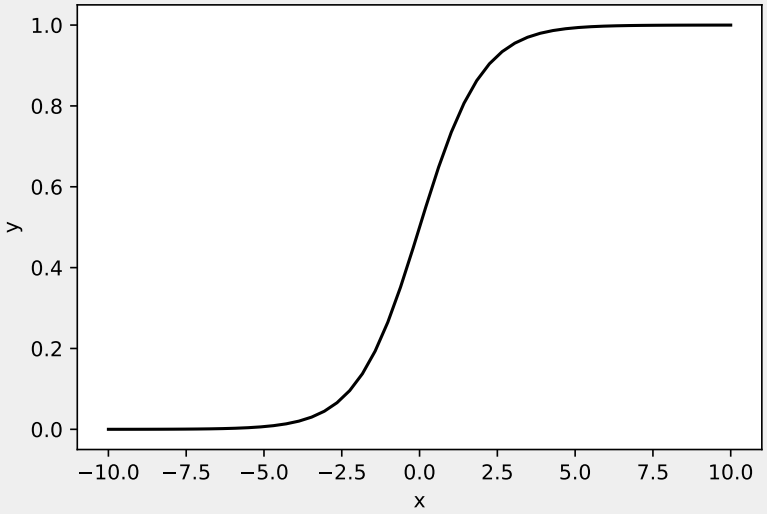
Logistic regression

- We convert $x^\top \theta$ to probabilities

$$\mathbb{P}(\, Y = 1 \,|\, x) = \sigma(x^\top \theta)$$

- The function σ denotes the sigmoid function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



Logistic regression

- Given a training set (X, y) how do we estimate θ?
- Option 1: Minimizing squared error (similar to OLS)

$$\hat{\theta} = \arg\min_{\theta} \sum_{i=1}^{n} \left[y_i - \sigma(x_i^\top \theta) \right]$$

  Problem: Not convex!

- Remember how we justified OLS for linear models?
- Option 2: Maximum likelihood

$$\hat{\theta} = \arg\max_{\theta} \mathbb{P}(y \mid X, \theta)$$

Logistic regression

- What is the probability of (X, y)?
- Remember a Bernoulli experiment (coin flip) with outcomes H (head) and T (tail)
- H is observed with probability p
- T is observed with probability $1 - p$
- The sequence HHTHT has probability

$$\mathbb{P}(\mathrm{HHTHT}) = pp(1-p)p(1-p)$$

- Remember the following rule of thumb:

$$\times = \text{"and"}$$
$$+ = \text{"or"}$$

Logistic regression

- For logistic regression, assume $y = (1, 1, 0, 1)$, hence

$$\mathbb{P}(1, 1, 0, 1 \mid X, \theta) = \sigma(x_1^\top \theta)\sigma(x_2^\top \theta)(1 - \sigma(x_3^\top \theta))\sigma(x_4^\top \theta)$$

- Write it nicely in general form:

$$\mathbb{P}(y \mid X, \theta) = \prod_{i=1}^{n} \sigma(x_i^\top \theta)^{y_i}(1 - \sigma(x_i^\top \theta))^{1-y_i}$$

- Maximum likelihood

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} \prod_{i=1}^{n} \sigma(x_i^\top \theta)^{y_i}(1 - \sigma(x_i^\top \theta))^{1-y_i} \\ &= \arg\max_{\theta} \sum_{i=1}^{n} y_i \log \sigma(x_i^\top \theta) + (1 - y_i) \log(1 - \sigma(x_i^\top \theta))\end{aligned}$$

- Convex optimization problem, but must be solved numerically

Learning goals

- Understand linear regression and the probabilistic foundation between regression models.
  - OLS is the Maximum a Posteriori / Maximum Likelihood of a linear relationship between input and target.
- Understand kernel regression when the relationship between features and outcome is not linear.
  - Kernel methods can account for non linear relationship with the kernel trick. It allows to understand many aspects of more complex models, such as neural networks
- Understand logistic regression for classification.
  - We can formulate binary classification as a regression problem on the separating hyperplane, with a probabilistic formulation. We will see many learning problem can be reformulated in a regression framework.

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