

MACHINE LEARNING IN BIOINFORMATICS

FROM LINEAR REGRESSION TO KERNEL REGRESSION

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LINEAR REGRESSION

- Solid understanding of linear regression allows us to understand many aspects of complex models, including neural networks
- Many models can be derived from linear regression, including polynomial, kernel, and logistic regression, as well as neural networks
- We start from a Bayesian perspective and show how to derive the linear regression model and a method for parameter estimation with a specific focus on model assumptions

BAYES THEOREM

- Bayes theorem:

$$\text{pr}(H | X) = \frac{\text{pr}(X | H)\text{pr}(H)}{\text{pr}(X)}$$

where $\text{pr}(H | X)$ is the posterior distribution of a hypothesis H given observed data X , $\text{pr}(X | H)$ the likelihood, $\text{pr}(H)$ the prior distribution, and $\text{pr}(X)$ the marginal likelihood

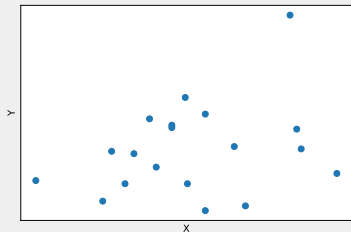
- H is our hypothesis and can take many forms, e.g.

- ▶ In case of the spam classifier we had $H = \text{'spam'}$
- ▶ H can also refer to the parameter of a distribution, e.g. when we want to estimate the mean of a normal distribution

- In any case, probabilities depend on our model assumptions and therefore are a subjective choice

LINEAR REGRESSION

Let **Y** be the dependent variable (response variable) and **X** the independent variable (covariate, or predictor):



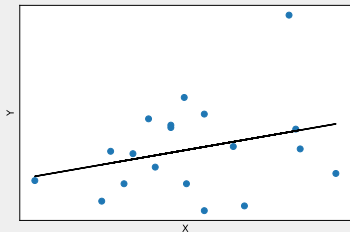
We assume the following model

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

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

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LINEAR REGRESSION

- We can also write $\mathbf{Y} \sim \text{Normal}(f(\mathbf{X}), \sigma^2)$
- 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 $i = 1, \dots, n$:
 - Select some value for x_i
 - Draw ϵ_i from $\text{Normal}(0, \sigma^2)$
 - 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 $y = (y_i)_{i=1}^n$
- An estimate $\hat{\theta}$ of our parameters θ can be computed as the *maximum a posterior (MAP) estimate*

$$\hat{\theta} = \arg \max_{\theta} \text{pr}(\theta | x, y)$$

- 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.

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

assuming $\text{pr}(\theta)$ is constant¹

- This result is not specific to linear regression models

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

LINEAR REGRESSION - PARAMETER ESTIMATION

- Furthermore, we have

$$\begin{aligned}\hat{\theta} &= \arg \max_{\theta} \text{pr}(\mathbf{x}, \mathbf{y} \mid \theta) \\ &= \arg \max_{\theta} \text{pr}(\mathbf{y} \mid \mathbf{x}, \theta) \text{pr}(\mathbf{x} \mid \theta) \\ &= \arg \max_{\theta} \text{pr}(\mathbf{y} \mid \mathbf{x}, \theta)\end{aligned}$$

- In the last step we took advantage of the fact that the distribution of our covariates \mathbf{x} does not depend on the parameters θ , which are the slope and intercept of the linear function
- In fact, we do not have to assume a particular distribution for our covariates!

LINEAR REGRESSION - OLS

- Plugging in our normal distribution we arrive at

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

- The estimate

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

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

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

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

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

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

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

LINEAR REGRESSION - NOTATION

- In general, we have n observations and p predictors
- For the i th 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. $\text{rank}(X) = \min(n, p)$

LINEAR REGRESSION - OLS

If $n > p$ and $X^T X$ 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:

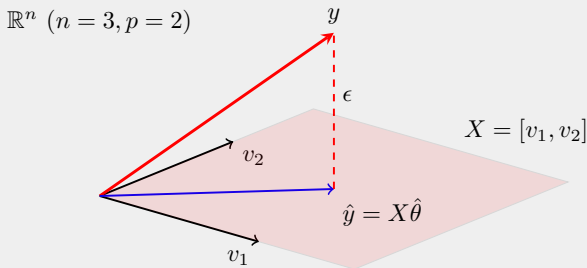
$$\begin{aligned} \Rightarrow \quad \hat{\theta} &= (X^T X)^{-1} X^T y \\ &= X^T y \quad \text{if } X^T X = I \end{aligned}$$

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

LINEAR REGRESSION - OLS PROJECTION

Let $X\theta = v_1\theta_1 + v_2\theta_2 + \dots v_p\theta_p$, where v_i denotes the i th 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

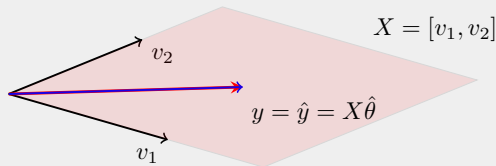
¹[Hastie et al., 2009]

LINEAR REGRESSION - OLS PROJECTION

Let $X\theta = v_1\theta_1 + v_2\theta_2 + \dots v_p\theta_p$, where v_i denotes the i th 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 $\epsilon = 0$

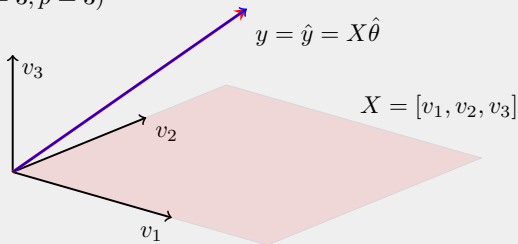
¹[Hastie et al., 2009]

LINEAR REGRESSION - OLS PROJECTION

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

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

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



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]

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 $\|y - X\hat{\theta}\|_2^2 = 0$!

LINEAR REGRESSION - UNDERDETERMINED OLS

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- Which one should we choose?

LINEAR REGRESSION - UNDERDETERMINED OLS

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

- 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

- For $p > n$ the OLS estimate

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

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

- 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** solution²

$$\begin{aligned} \arg \min_{\theta} \quad & \|\theta\|_2^2 \\ \text{subject to} \quad & X\theta = y \end{aligned}$$

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 pseudoinverse³ of $X^\top X$.

²**Common practice for training neural networks**

³The 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:

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

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

³Convex optimization: [Boyd and Vandenberghe, 2004]

LINEAR REGRESSION - RIDGE REGRESSION

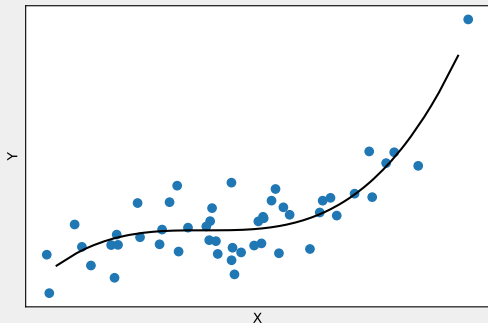
- For $\lambda \rightarrow \infty$ the estimate $\lambda \hat{\theta}(\lambda)$ converges to the componentwise regression estimator
- For $\lambda \rightarrow 0$ the estimate $\hat{\theta}(\lambda)$ converges to the minimum ℓ_2 -norm OLS solution⁴
- The penalty $\lambda \|\theta\|_2^2$ can be interpreted 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 **X** and **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 $\phi : \mathbb{R}^p \rightarrow \mathbb{R}^{p'}$ 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.

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 $\theta \in \text{span}(\phi(x_1), \dots, \phi(x_n)) \subset \mathbb{R}^p$. 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 $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called a *kernel* if there exists a feature map $\phi : \mathcal{X} \rightarrow \mathcal{F}$ such that

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

$K = (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{\mathbf{x}_i \in \mathcal{X}, \mathbf{x}_j \in \mathcal{X}}$ is called the kernel matrix.

- \mathcal{X} can be an arbitrary space, for instance DNA sequences
- $\kappa(\mathbf{x}_i, \mathbf{x}_j)$ is interpreted as a similarity measure in feature space
- Evaluating $\kappa(\mathbf{x}_i, \mathbf{x}_j)$ does not always require to explicitly compute $\phi(\mathbf{x})$
- 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 $d = 2$

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

■ 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)

RANDOM FEATURES

RANDOM FEATURES

Kernel matrix grows quadratically with the number of data points, which prevents kernel methods to be applied to large data sets.

Basic idea⁵: Define a mapping $\xi : \mathcal{X} \rightarrow \mathbb{R}^q$ with $q \ll p$ such that

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j) \approx \xi(\mathbf{x}_i)^\top \xi(\mathbf{x}_j)$$

Regression can then be performed in \mathbb{R}^q after explicitly mapping each data point to the reduced feature space.

How do we compute ξ ?

⁵[Rahimi et al., 2007]

Bochner's theorem

A continuous shift-invariant kernel $\kappa : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C}$ with $\kappa(x_i, x_j) = \kappa(x_i - x_j)$ is positive definite iff there exists a non-negative measure μ such that

$$\begin{aligned}\kappa(x_i - x_j) &= \int_{\mathbb{R}^d} \exp(i\omega^\top (x_i - x_j)) \, d\mu(\omega) \\ &= \mathbb{E}_\omega \exp(i\omega^\top (x_i - x_j)) = \mathbb{E}_\omega \exp(i\omega^\top x_i) \exp(i\omega^\top x_j)^* .\end{aligned}$$

I.e. the kernel κ is the (inverse) Fourier transform of μ .

When both κ and μ are real-valued then

$$\kappa(x_i - x_j) = \mathbb{E}_\omega \cos(\omega^\top (x_i - x_j))$$

⁵ x^* is the complex conjugate of x and remember that $\exp(ix)^* = \exp(-ix)$

Monte Carlo approximation

Let μ be a distribution and ω a random variable with distribution μ . From the law of large numbers it follows that

$$\mathbb{E}_{\omega} f(\omega) = \int f(x) d\mu(x) \approx \frac{1}{q} \sum_{j=1}^q f(\omega_j)$$

where $\omega_1, \dots, \omega_q$ are independent samples from μ .

Monte Carlo approximation of the Fourier integral

$$\omega_k \stackrel{i.i.d.}{\sim} \mu$$

$$\kappa(x_i, x_j) \approx \frac{1}{q} \sum_{k=1}^q \exp(i\omega_k^\top (x_i - x_j)) = \xi(x_j)^* \xi(x_i)$$

where $\xi(x) = \frac{1}{\sqrt{q}} (\exp(i\omega_1^\top x), \dots, \exp(i\omega_q^\top x))^\top$.

RANDOM FEATURES

In practice: We know the kernel κ and must derive the measure μ . Afterwards, we can approximate κ by drawing q samples ω_k from μ and map x into feature space using

$$\xi(x) = \frac{1}{\sqrt{q}} \left(\exp(i\omega_1^\top x), \dots, \exp(i\omega_q^\top x) \right)^\top.$$

The measure μ is given by the Fourier transform of κ with density

$$f_\mu(\omega) = \int_{\mathbb{R}^d} \exp(-i\omega^\top \delta) \kappa(\delta) d\delta, \quad \text{where} \quad \delta = x_i - x_j$$

RANDOM FEATURES

Example: Radial basis function (RBF) kernel (infinite dimensional feature space)

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

The measure μ is given by a spherical normal distribution ($\Sigma = \sigma^2 I$) with density

$$f_\mu(\omega) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{\|\omega\|_2^2}{2\sigma^2}\right)$$

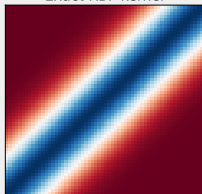
Since κ and μ are real, we have

$$\xi(x) = \frac{1}{\sqrt{q}} \left(\cos(\omega_1^\top x), \sin(\omega_1^\top x), \dots, \cos(\omega_q^\top x), \sin(\omega_q^\top x) \right)^\top$$

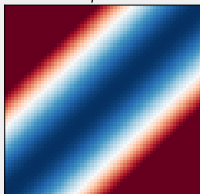
⁵ $\cos(x_i - x_j) = \cos(x_i)\cos(x_j) + \sin(x_i)\sin(x_j)$

RANDOM FEATURES

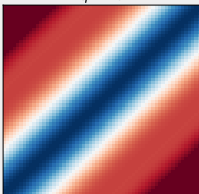
Exact RBF kernel



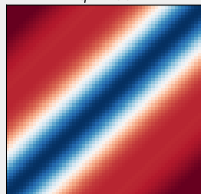
$q = 1$



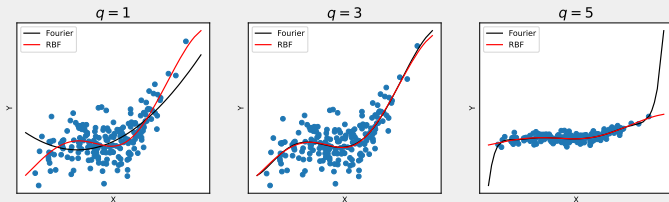
$q = 10$



$q = 100$

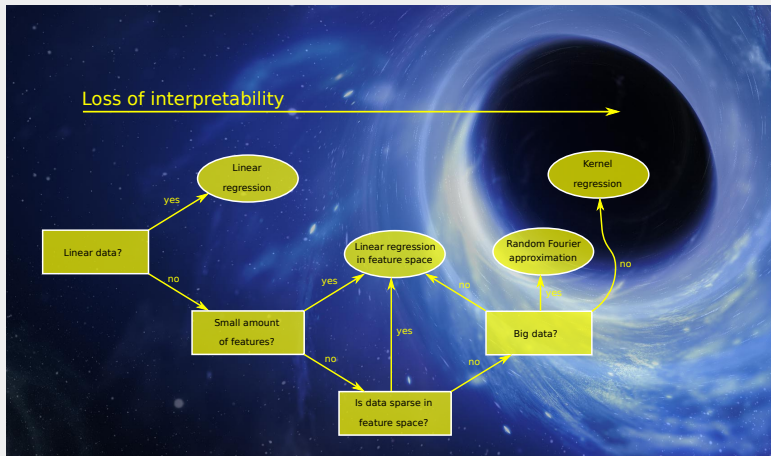


RANDOM FEATURES






- Kernel regression is not identical to linear regression with random Fourier features
- As many parameters as random Fourier features
- Regularization must be used to prevent overfitting

GUIDE TO KERNEL REGRESSION



⁵The complexity of kernel regression can be reduced by computing approximate solutions with batch gradient descent

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