

Large Scale Machine Learning

Introduction

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Acknowledgement

Slides inspired by

- Chloé-Agathe Azencott
- Jean-Philippe Vert
- Claire Boyer

Why machine learning ?

A brief zoo of ML problems

- Dimension reduction: PCA

- Clustering: k -means

- Regression: ridge regression

- Classification: logistic regression and SVM

- Nonlinear models: kernel methods

Algorithmic complexity recap

2017 is the year of Machine Learning. Here's why

■ GAURAV SANGWANI

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| JAN 13, 2017, 12:51 PM

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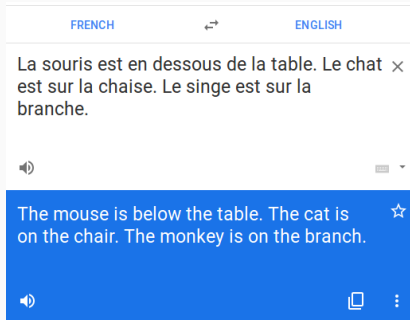
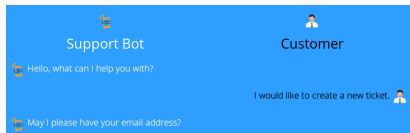


Machine learning is maybe the most sweltering thing in Silicon Valley at this moment. Particularly deep learning. The reason why it is so hot is on the grounds that it can assume control of numerous repetitive, thoughtless tasks. It'll improve doctors, and make lawyers better lawyers. What's more, it makes cars drive themselves.

Perception

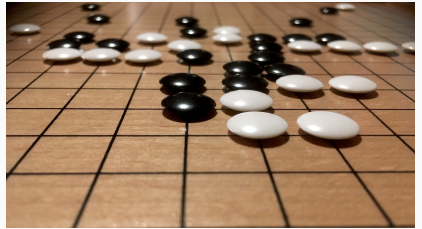
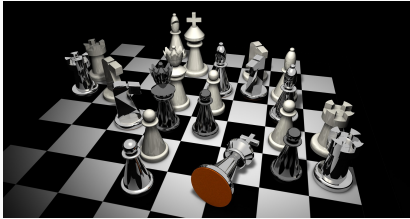


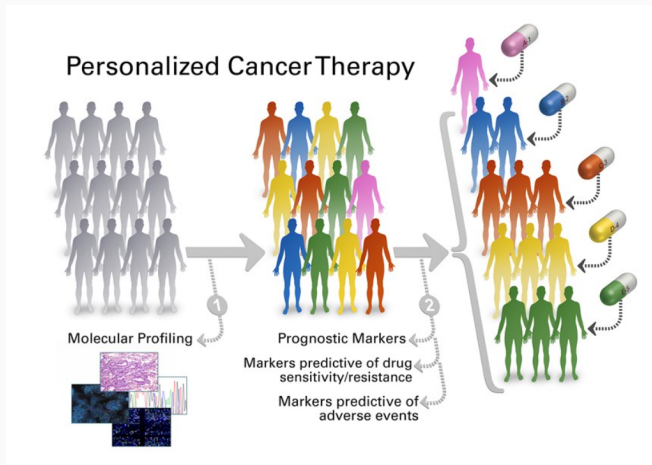
Communication





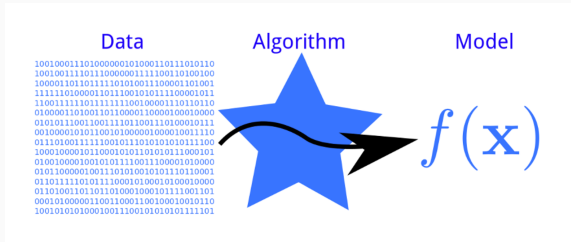
Reasoning





<https://pct.mdanderson.org>

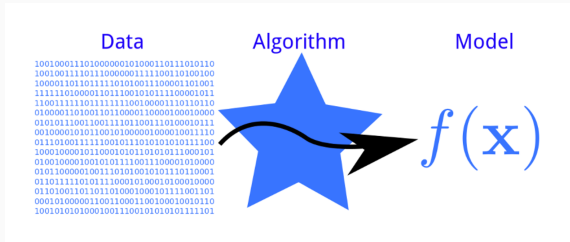
A common process: learning from data



<https://www.linkedin.com/pulse/supervised-machine-learning-pegadecisioning-solution-nizam-muhammad>

- Given examples (training data), make a machine learn how to predict on new samples, or discover patterns in data

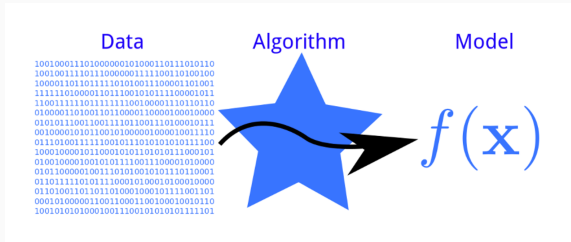
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- Statistics + optimization + computer science

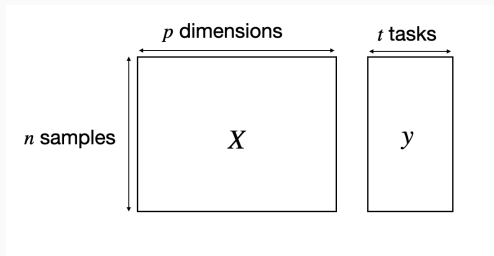
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- Given examples (training data), make a machine learn how to predict on new samples, or discover patterns in data
- Statistics + optimization + computer science
- Gets better with more training examples and bigger computers

Large-scale ML?



- Iris dataset: $n = 150, p = 4, t = 1$
- Cancer drug sensitivity: $n = 10^3, p = 10^6, t = 100$
- Imagenet: $n = 14 \cdot 10^6, p = 60 \cdot 10^3, t = 22 \cdot 10^3$
- Shopping, e-marketing $n = \mathcal{O}(10^6), p = \mathcal{O}(10^9), t = \mathcal{O}(10^8)$
- Astronomy, GAFAMS, web... $n = \mathcal{O}(10^9), p = \mathcal{O}(10^9), t = \mathcal{O}(10^9)$

Today's goals

1. Review a few standard ML techniques
2. Introduce a few ideas and techniques to scale them to modern, big datasets

Why machine learning ?

A brief zoo of ML problems

Dimension reduction: PCA

Clustering: k -means

Regression: ridge regression

Classification: logistic regression and SVM

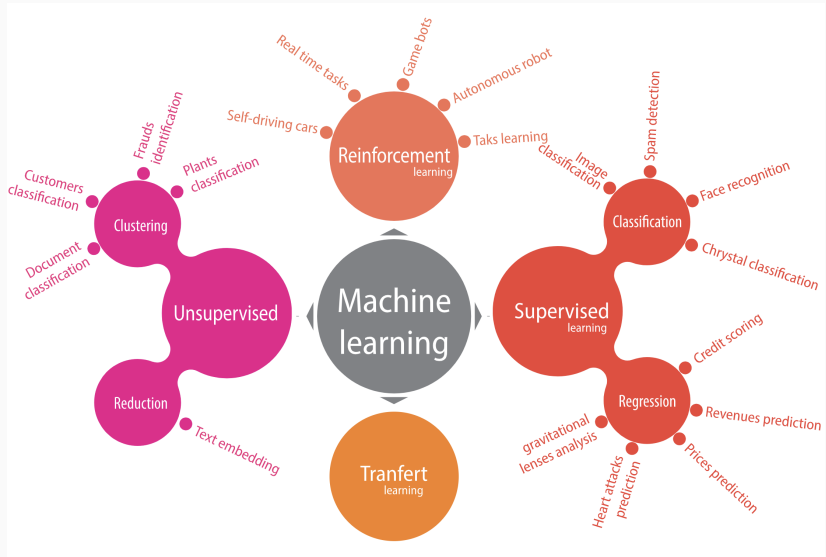
Nonlinear models: kernel methods

Algorithmic complexity recap

ML develops generic methods for solving different types of problems:

- **Supervised** learning
Goal: learn from examples
- **Unsupervised** learning
Goal: learn from data alone, extract structure in the data
- **Reinforcement** learning
Goal: learn by exploring the environment (e.g. games or autonomous vehicle)

Learning scenarios



Unsupervised learning

Clustering :

Finding Common Relationships



What is the relationship between these data ?

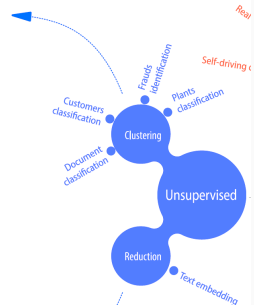


Simplify while keeping meaning



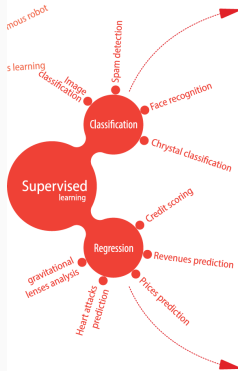
Reduction :

Reduce the number of dimensions



source: fidle-cnrs

Supervised learning



Classification :

Predict qualitative informations



This is a cat



This is a rabbit



Tell me,
what is it ?



Régression :

Predict quantitative informations



150 K€



400 K€



120 K€



100 K€



Tell me,
what's the
price ?



source: fidle-cnrs

Main ML paradigms

- Unsupervised learning
 - Dimension reduction
 - Clustering
 - Density estimation
 - Feature learning
- Supervised learning
 - Regression
 - Classification
 - Structured output classification
- Semi-supervised learning
- Reinforcement learning

Main ML paradigms

- Unsupervised learning
 - Dimension reduction: PCA
 - Clustering: k-means
 - Density estimation
 - Feature learning
- Supervised learning
 - Regression: OLS, ridge regression
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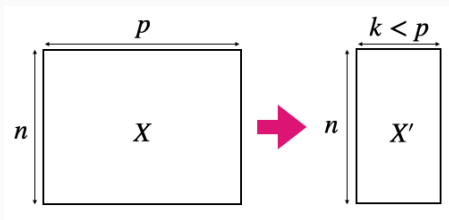
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Algorithmic complexity recap

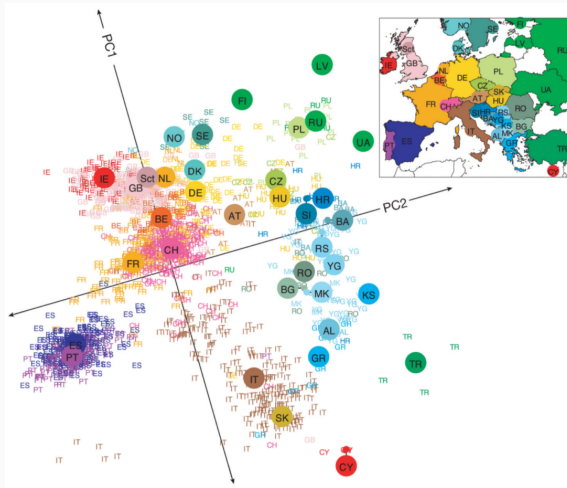
Motivation



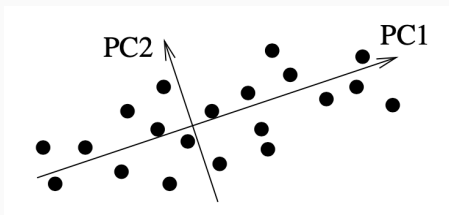
- Reduce the dimension without losing the variability in the data;
- Visualization ($k = 2, 3$)
- Discover structure

Motivation: Population genetics

- Genetic data of 1387 Europeans

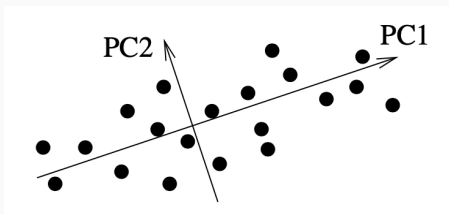


PCA definition



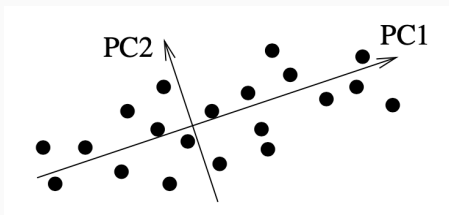
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PCA definition



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 - Is orthogonal to all previous components:

$$\langle w_k, w_1 \rangle = \langle w_k, w_2 \rangle = \dots = \langle w_k, w_{k-1} \rangle = 0$$



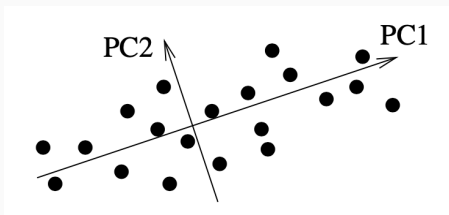
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- Captures the largest amount of variance:

$$\max_{\|w\|=1} w^\top X^\top X w = \max_{\|w\|=1} \|Xw\|^2$$

($X^\top X$: empirical covariance of X (centered))



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- **Solution:** w is the k th eigenvector of $X^\top X$.

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Example

$$n = 10^9, p = 10^8$$

- Store $X^\top X$: 10^{16} B = 9000 TB
- Compute $X^\top X$: 10^{25} FLOPS

A US Supercomputer Just Broke The Exascale Barrier, Ranking Fastest in The World

TECH 07 June 2022 By PETER DOCKRILL



Frontier. ([Oak Ridge National Laboratory/YouTube](#))

The US has succeeded in developing the world's first 'true' exascale supercomputer, honoring a [pledge made by President Obama](#) almost seven years ago, and ushering the world into a new era of computational capability.

Until now, the most speedy supercomputers in the world were still working in the petascale, achieving a quadrillion calculations per second. The exascale brings this to a whole new level, [reaching a quintillion operations per second](#).

The [Frontier supercomputer](#), built at the Department of Energy's Oak Ridge National Laboratory in Tennessee, has now become the world's first known supercomputer to demonstrate a processor speed of 1.1 exaFLOPS (1.1 quintillion floating point operations per second, or [FLOPS](#)).

PCA complexity

- **Memory:** store X and covariance matrix $X^\top X$: $\mathcal{O}(\max(np, p^2))$
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- Compute $X^\top X$: **10^{25} FLOPS** (Floating Point Operations per Second)

World's fastest computer (2022): 1.1 exaFLOPS = 10^{18} FLOPS
→ **115 days!**

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Clustering: k -means

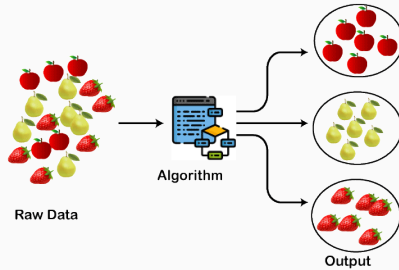
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Algorithmic complexity recap

Motivation



- Unsupervised learning
- Discover groups
- Reduce dimension

k -means definition

- Dataset $\{x^1, \dots, x^n\} \subset \mathbb{R}^p$.

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$$\boldsymbol{\mu}_j = \frac{1}{|\{i : c_i = j\}|} \sum_{i: c_i=j} \mathbf{x}^i$$

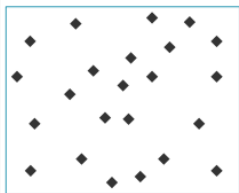
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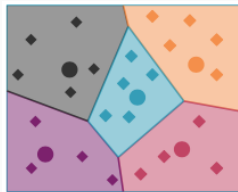
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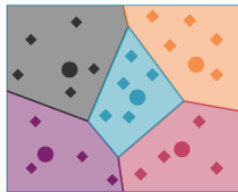
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→ Voronoi diagram

- NP-hard problem!

- **NP-hard problem!** Approximate solution by iterating
 1. **Assignment step:** fix the centroids μ_j , optimize assignments c_i

$$\forall i = 1, \dots, n, \quad c_i \leftarrow \operatorname{argmin}_{c \in \{1, \dots, k\}} \|x^i - \mu_c\|$$

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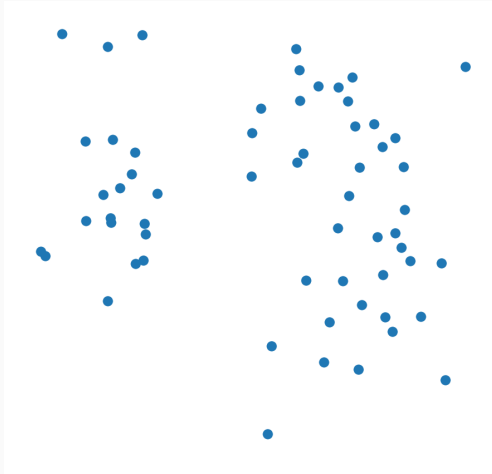
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2. **Update step:** update the centroids

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k -means example

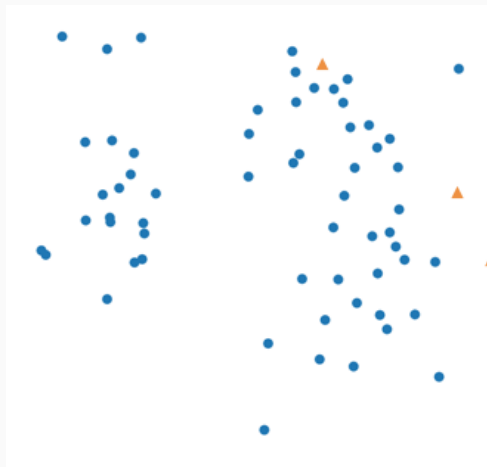
$$k = 3$$



k -means example

▷ Pick 3 centroids at random.

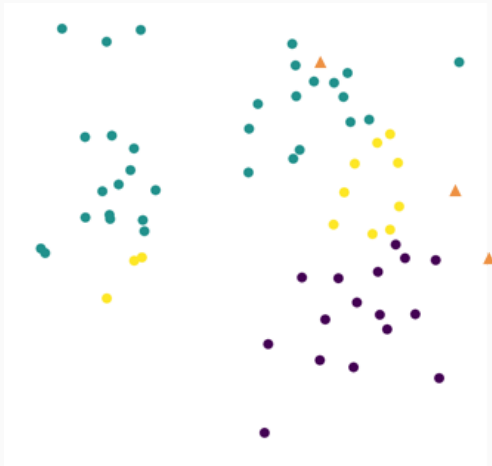
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k -means example

▷ Assign each observation to the nearest centroid

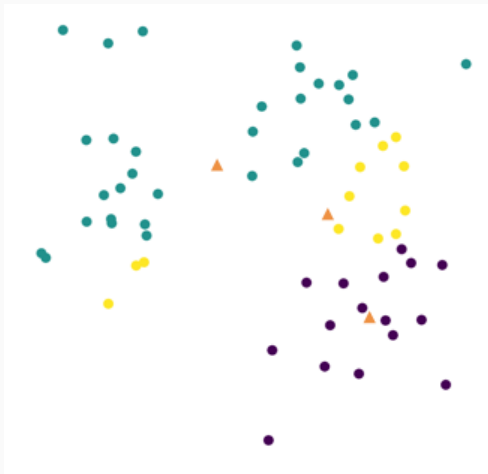
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k -means example

▷ Recompute centroids

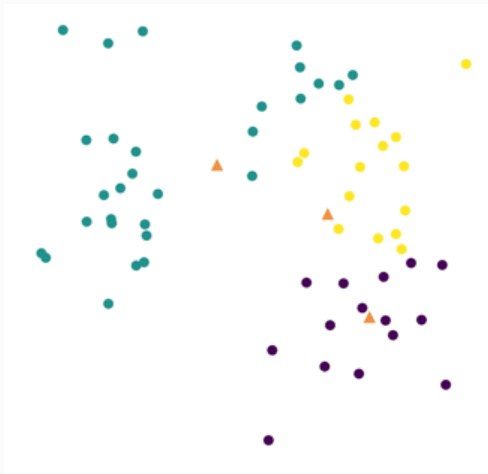
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k -means example

▷ Re-assign each observation to the nearest centroid

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k -means example

- ▷ Recompute centroids, and iterate process until convergence

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k -means complexity

- Runtime:

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- Do T iterations: $\mathcal{O}(kTnp)$

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- Store X : $\mathcal{O}(np)$

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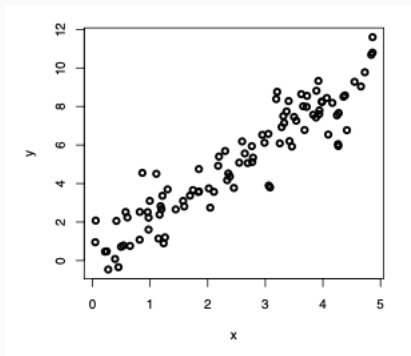
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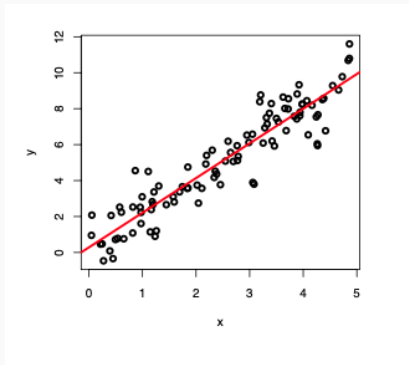
Algorithmic complexity recap

Motivation



- Predict a continuous output $y \in \mathbb{R}$ from an input $x \in \mathbb{R}^p$

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Linear regression

- Dataset:

$$\mathcal{S} = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)\} \subset \mathbb{R}^p \times \mathbb{R} \Leftrightarrow X \in \mathbb{R}^{n \times p}, \mathbf{y} \in \mathbb{R}^n$$

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- Fit a linear function:

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- Goodness of fit measured by residual sum of squares:

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Linear regression

- Dataset:

$$\mathcal{S} = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)\} \subset \mathbb{R}^p \times \mathbb{R} \Leftrightarrow X \in \mathbb{R}^{n \times p}, \mathbf{y} \in \mathbb{R}^n$$

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- Solution:

$$\hat{\boldsymbol{\beta}}^{\text{OLS}} = (X^\top X)^{-1} X^\top \mathbf{y}$$

(uniquely defined when $X^\top X$ invertible)

Ridge regression

- Hoerl and Kennard, [1970](#)
- Ridge regression minimizes the **regularized** RSS:

$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\operatorname{argmin}} \operatorname{RSS}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

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- Solution:

$$\hat{\beta}^{\text{ridge}} = (X^{\top} X + \lambda I)^{-1} X^{\top} \mathbf{y}$$

→ *unique and always exists !*

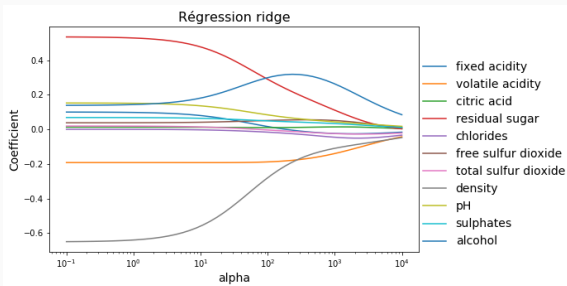
- Correlated features get similar weights

Limit cases

$$\hat{\beta}_{\lambda}^{\text{ridge}} = (X^{\top} X + \lambda I)^{-1} X^{\top} y$$

Corollary

- As $\lambda \rightarrow 0$, $\hat{\beta}_{\lambda}^{\text{ridge}} \rightarrow \hat{\beta}^{\text{OLS}}$ (low bias, high variance).
- As $\lambda \rightarrow +\infty$, $\hat{\beta}_{\lambda}^{\text{ridge}} \rightarrow 0$ (high bias, low variance).



$$\hat{\beta}_{\lambda}^{\text{ridge}} = (X^{\top} X + \lambda I)^{-1} X^{\top} \mathbf{y}$$

- Compute $X^{\top} X + \lambda I$: $\mathcal{O}(np^2)$

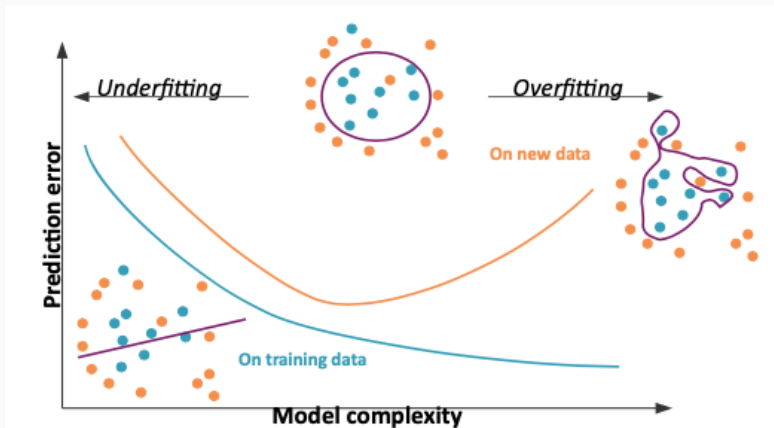
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 - Split the training set (of size n) into K equally-sized chunks

Valid	Training	
Valid		Training
Training	Valid	
Training		Valid

Choice of λ

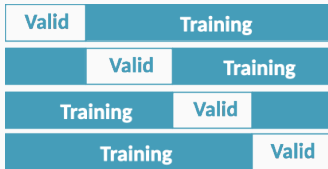
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- Multiplies complexity by **KM** !

Generalization: ℓ_2 -regularized learning

- Generalization of the ridge regression to any **loss**:

$$\min_{\boldsymbol{\beta}} \frac{1}{n} \sum_{i=1}^n \ell(f_{\boldsymbol{\beta}}(\mathbf{x}^i), y^i) + \lambda \|\boldsymbol{\beta}\|^2$$

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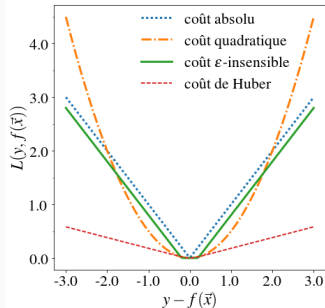
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Losses for regression

- Square loss : $\ell(u, y) = (u - y)^2$
→ *Ridge regression*
- Absolute loss: $\ell(u, y) = |u - y|$
- ϵ -insensitive loss :
 $\ell(u, y) = (|u - y| - \epsilon)_+$
- Huber loss : mix quadratic/linear

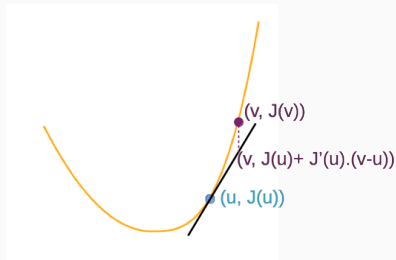


Gradient descent

If the loss is *convex*, then the problem is *strictly convex* and has a *unique global solution*, which can be found *numerically*.

- Assume the function to minimize is differentiable, then

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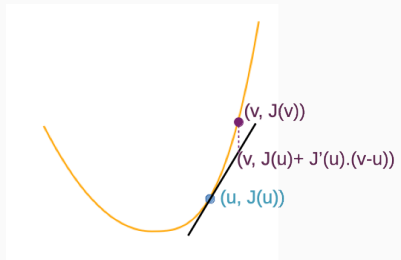
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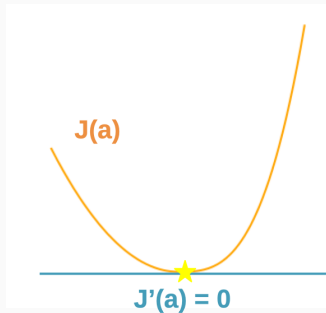
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- $\nabla J(u) = 0 \Leftrightarrow u$ minimizes J



Gradient descent

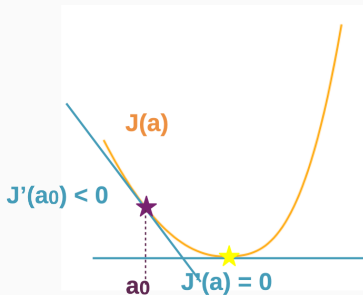
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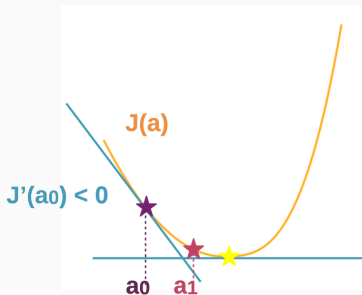


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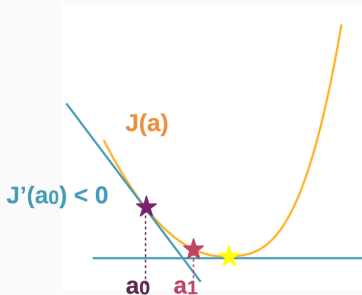


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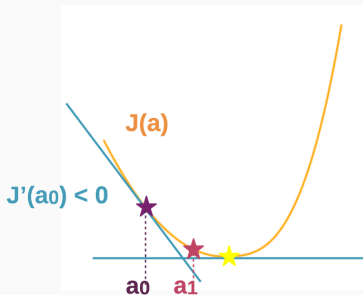


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- Stop when $|\nabla J(a_0)| < \varepsilon$



Why machine learning ?

A brief zoo of ML problems

Dimension reduction: PCA

Clustering: k -means

Regression: ridge regression

Classification: logistic regression and SVM

Nonlinear models: kernel methods

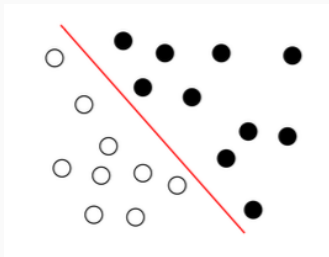
Algorithmic complexity recap

Motivation



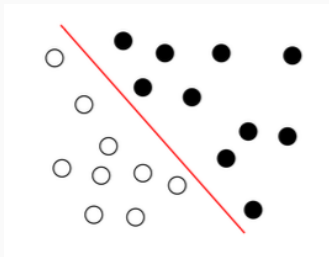
- Predict the category of data
- 2 or more (sometimes many) categories

Linear models for classification



- Training set $\mathcal{S} = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^n, y^n)\} \subset \mathbb{R}^p \times \{-1, 1\}$

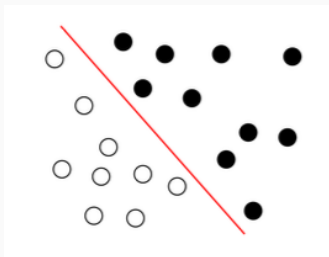
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$$f_{\beta}(\mathbf{x}) = \beta^{\top} \mathbf{x}$$

- Prediction on a new point $\mathbf{x} \in \mathbb{R}^p$:

$$\begin{cases} +1 & \text{if } f_{\beta}(\mathbf{x}) > 0, \\ -1 & \text{otherwise.} \end{cases}$$

The 0/1 loss

- The 0/1 loss measures if a prediction is correct or not:

$$\ell_{0/1}(f(\mathbf{x}), y) = \mathbb{1}(yf(\mathbf{x}) < 0) = \begin{cases} 0 & \text{if } y = \text{sign}(f(\mathbf{x})) \\ 1 & \text{otherwise.} \end{cases}$$

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- However:
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 - The regularization has **no effect** since the 0/1 loss is invariant by scaling of β

The logistic loss

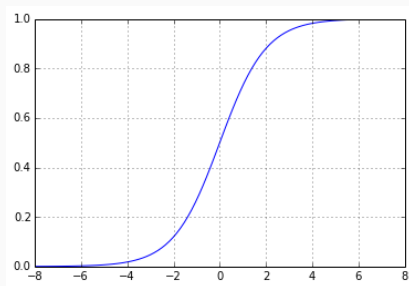
- An alternative is to define a **probabilistic model** of y parametrized by $f(\mathbf{x})$, e.g.:

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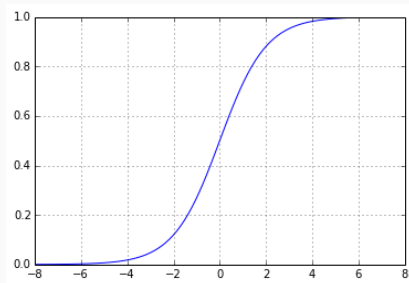
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- The **logistic loss** is the negative conditional likelihood:

$$\ell_{\text{logistic}}(f(\mathbf{x}), y) = -\ln p(y | f(\mathbf{x})) = \ln(1 + e^{-yf(\mathbf{x})})$$

- Cessie and Houwelingen ([1992](#))

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- Take $\alpha = (\nabla^2 J(u^{\text{old}}))^{-1}$ in the gradient step

Solving ridge logistic regression

$$\min_{\boldsymbol{\beta}} J(\boldsymbol{\beta}) = \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-y^i \boldsymbol{\beta}^\top \mathbf{x}^i}) + \lambda \|\boldsymbol{\beta}\|_2^2$$

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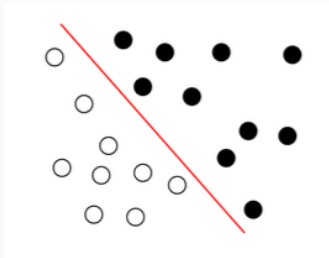
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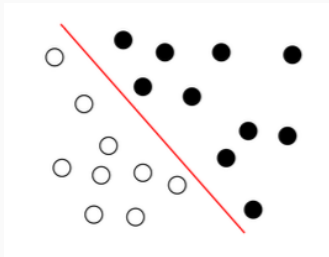
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- Complexity $\mathcal{O}(T(np^2 + p^3))$

Large-margin classifiers



- For any $f : \mathbb{R}^p \rightarrow \mathbb{R}$, the **margin** of f on an (x, y) pair is $yf(x)$

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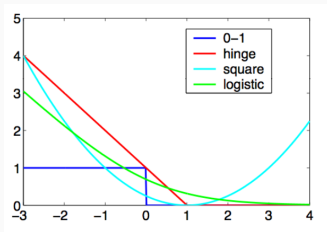
$$yf(\mathbf{x})$$

- Large-margin classifiers: maximize $yf(\mathbf{x})$

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^n \phi(y^i f_{\boldsymbol{\beta}}(\mathbf{x}^i)) + \lambda \boldsymbol{\beta}^{\top} \boldsymbol{\beta}$$

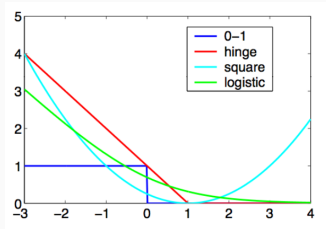
for a **convex, non-increasing** function $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$

Loss function examples



Loss	Method	$\phi(u)$
0-1	none	$1(u \leq 0)$
Hinge	Support vector machine (SVM)	$\max(1 - u, 0)$
Logistic	Logistic regression	$\log(1 + e^{-u})$
Square	Ridge regression	$(1 - u)^2$
Exponential	Boosting	e^{-u}

Which ϕ ?



- Computation
 - ϕ convex means we need to solve a convex optimization problem.
 - A "good" ϕ may be one which allows for fast optimization
- Theory
 - Most ϕ lead to consistent estimators
 - Some may be more efficient

- Boser et al. (1992)

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^n \max(0, 1 - y^i \boldsymbol{\beta}^\top \mathbf{x}^i) + \lambda \|\boldsymbol{\beta}\|^2$$

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- **Memory:** $\mathcal{O}(n^2)$ to store XX^\top

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- **Memory:** $\mathcal{O}(n^2)$ to store XX^\top
- **Runtime:** $\mathcal{O}(n^3)$ to find α^*

Complexity (prediction)

- **Primal:** $\mathcal{O}(p)$ for $(\beta^*)^\top \mathbf{x}$

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- **Runtime:** $\mathcal{O}(n^3)$ to find α^*

Complexity (prediction)

- **Primal:** $\mathcal{O}(p)$ for $(\beta^*)^\top \mathbf{x}$
- **Dual:** $\mathcal{O}(np)$ for $(\alpha^*)^\top X \mathbf{x}$

Why machine learning ?

A brief zoo of ML problems

Dimension reduction: PCA

Clustering: k -means

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Classification: logistic regression and SVM

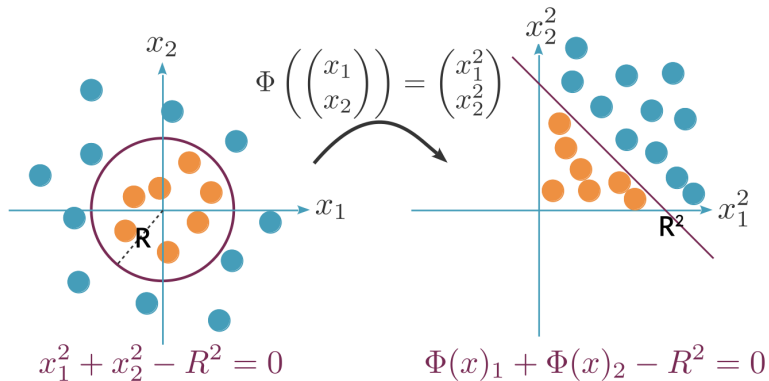
Nonlinear models: kernel methods

Algorithmic complexity recap

Motivation



Non-linear mapping to a feature space



$$\phi : \mathbb{R}^p \rightarrow \mathcal{H}$$

- Training:

$$\max_{\alpha \in \mathbb{R}^n} 2 \sum_{i=1}^n \alpha_i - \sum_{j,k=1}^n \alpha_j \alpha_k y^j y^k (\mathbf{x}^j{}^\top \mathbf{x}^k)$$

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- Predict with the decision function

$$f_{\beta^*}(x) = \sum_{j=1}^n \alpha_j y^j \mathbf{x}^j{}^\top x$$

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$$k : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}$$

$$(x, x') \mapsto k(x, x') = \langle \phi(x), \phi(x') \rangle$$

- Training:

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- k may be quite **efficient** to compute, even if \mathcal{H} is a very **high-dimensional** or even infinite-dimensional space.

Kernel trick

- k may be quite **efficient** to compute, even if \mathcal{H} is a very **high-dimensional** or even infinite-dimensional space.
- For any **positive semi-definite** function k , there exists a feature space \mathcal{H} and a feature map ϕ such that

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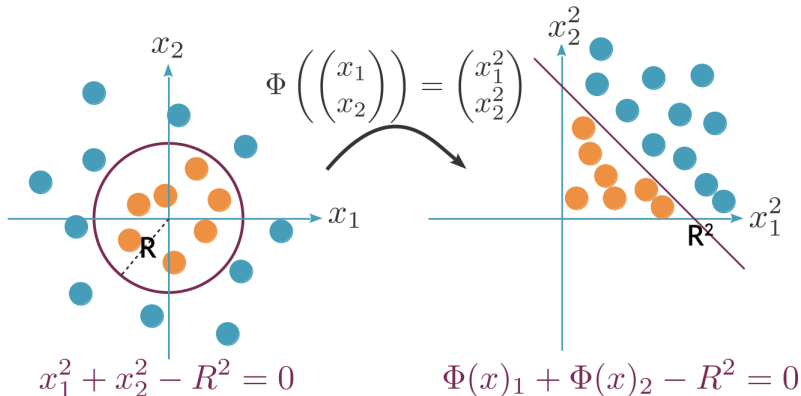
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- Hence you can define mappings **implicitly**.
- **Kernel trick**: algorithms that only involve the samples through their dot products can be rewritten using kernels in such a way that they can be applied in the initial space without ever computing the mapping ϕ .

Non-linear mapping to a feature space



$$K(\mathbf{x}, \mathbf{x}') = \left\langle \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \begin{pmatrix} x_1'^2 \\ x_2'^2 \end{pmatrix} \right\rangle = x_1^2 x_1'^2 + x_2^2 x_2'^2$$

Linear	$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$
Polynomial	$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + c)^d$
Gaussian	$k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{\ \mathbf{x} - \mathbf{x}'\ ^2}{2\sigma^2})$
Min/max	$k(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^p \frac{\min(x_j , x'_j)}{\max(x_j , x'_j)}$

Kernel ridge regression (KRR)

- Ridge regression in input space \mathbb{R}^p :

$$f_{\beta}(\mathbf{x}) = \mathbf{x}^{\top} \hat{\boldsymbol{\beta}}^{\text{ridge}} = \mathbf{x}^{\top} \underbrace{(\mathbf{X}^{\top} \mathbf{X} + \lambda \mathbf{I})^{-1}}_{p \times p} \mathbf{X}^{\top} \mathbf{y},$$

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- In a feature space of dimension \mathbb{R}^d :

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- Ridge regression in sample space \mathbb{R}^n :

$$f_{\beta}(\mathbf{x}) = \kappa \underbrace{(\mathbf{K} + \lambda \mathbf{I})^{-1}}_{n \times n} \mathbf{y}, \quad \kappa_i = k(\mathbf{x}, \mathbf{x}^i), \quad K_{ij} = k(\mathbf{x}^i, \mathbf{x}^j)$$

$$f_{\beta}(\mathbf{x}) = \kappa(K + \lambda I)^{-1} \mathbf{y}, \quad \kappa_i = k(\mathbf{x}, \mathbf{x}^i), \quad K_{ij} = k(\mathbf{x}^i, \mathbf{x}^j)$$

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Summary

Method	Memory	Training time	Test time
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- Test time: prediction should be fast!

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Techniques for large-scale ML

- Understand modern architecture, and how to distribute data / computation
- Trade optimization accuracy for speed
- Use the deep learning tricks

-  Boser, Bernhard E, Isabelle M Guyon, and Vladimir N Vapnik (1992). “A training algorithm for optimal margin classifiers”. In: *Proceedings of the fifth annual workshop on Computational learning theory*, pp. 144–152.
-  Cessie, S Le and JC Van Houwelingen (1992). “Ridge estimators in logistic regression”. In: *Journal of the Royal Statistical Society Series C: Applied Statistics* 41.1, pp. 191–201.
-  Hoerl, Arthur E and Robert W Kennard (1970). “Ridge regression: Biased estimation for nonorthogonal problems”. In: *Technometrics* 12.1, pp. 55–67.