Large Scale Machine Learning

Introduction to large-scale ML & optimization

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Acknowledgements

Slides inspired by:

- Adeline Fermanian
- Chloé-Agathe Azencott

Contents

TECH

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

GAURAV SANGWANI | 0 | JAN 13, 2017, 12.51 PM

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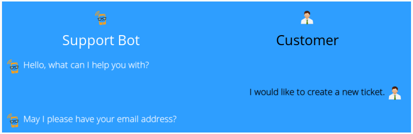
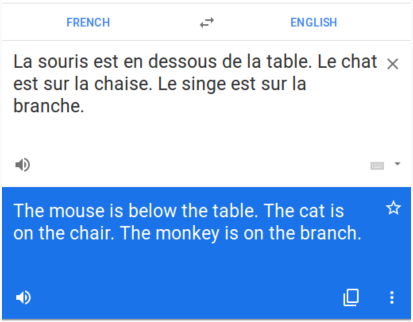
Machine learning is maybe the most sweltering thing in Silicon Valley at this moment. Particularly deep learning. The reason why it is so hot is on the grounds that it can assume control of numerous repetitive, thoughtless tasks. It'll improve doctors, and make lawyers better lawyers. What's more, it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

Perception

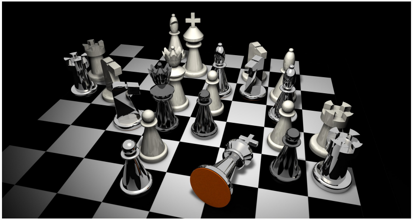
Communication

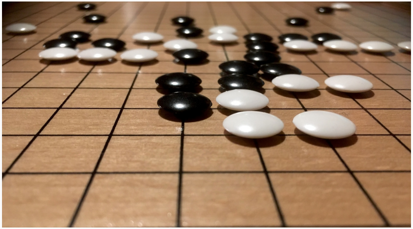




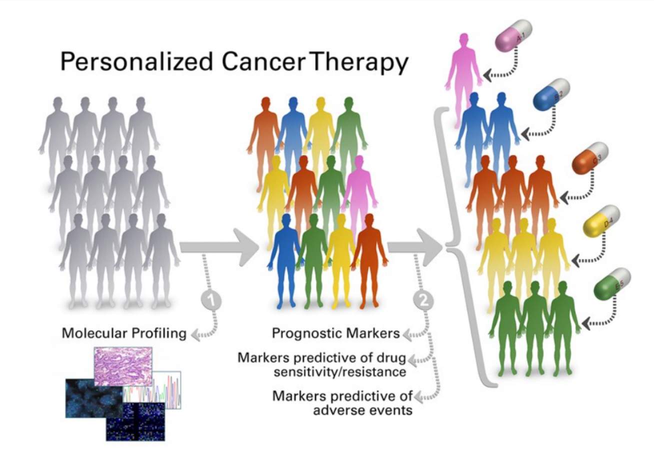
Mobility

Reasoning



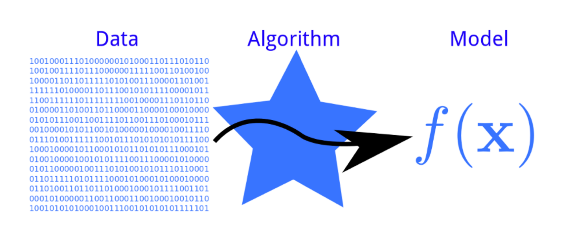


Health



https://pct.mdanderson.org

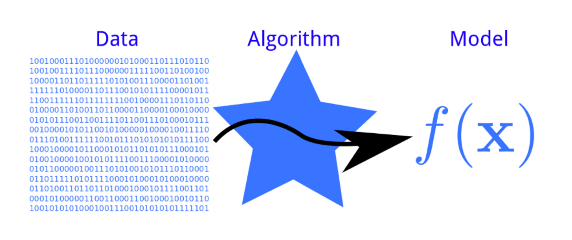
Learning from data



https://www.linkedin.com/pulse/supervised-machine-learning-pega-decisioning-solution-nizam-muhammad

- Given: examples (training data)
  Goal: predict on new samples, or discover patterns in data

Learning from data



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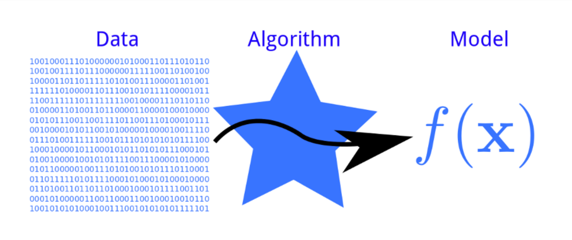

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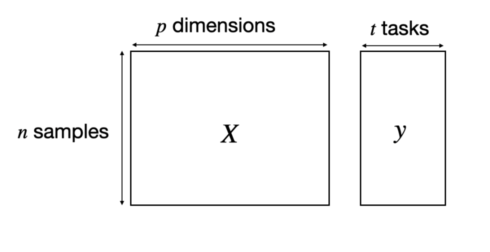
- Given: examples (training data)
  Goal: predict on new samples, or discover patterns in data
- Statistics + optimization + computer science
- Training gets better with more training examples and more powerful computers

Large-Scale Machine Learning



Dataset examples:

- Iris dataset: $n = 150$, $p = 4$, $t = 1$
- Cancer drug sensitivity: $n = 10^3$, $p = 10^6$, $t = 100$
- Imagenet: $n = 14.10^6$, $p = 60.10^3$, $t = 22.10^3$
- Shopping, e-marketing $n = \mathcal{O}(10^6)$, $p = \mathcal{O}(10^9)$, $t = \mathcal{O}(10^8)$
- Astronomy, GAFAMs, web... $n = \mathcal{O}(10^9)$, $p = \mathcal{O}(10^9)$, $t = \mathcal{O}(10^9)$

Objectives for this lecture

1. Review several standard ML methods

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2. Discuss complexity of these methods
3. Introduce some techniques to scale these methods to big/large datasets

Contents

Learning scenarios

ML develops generic methods for solving different types of problems:

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  Goal: learning from unlabeled data, exploring structure of the data

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  Goal: learning by exploring the environment (e.g. games or autonomous vehicle)

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- Supervised learning
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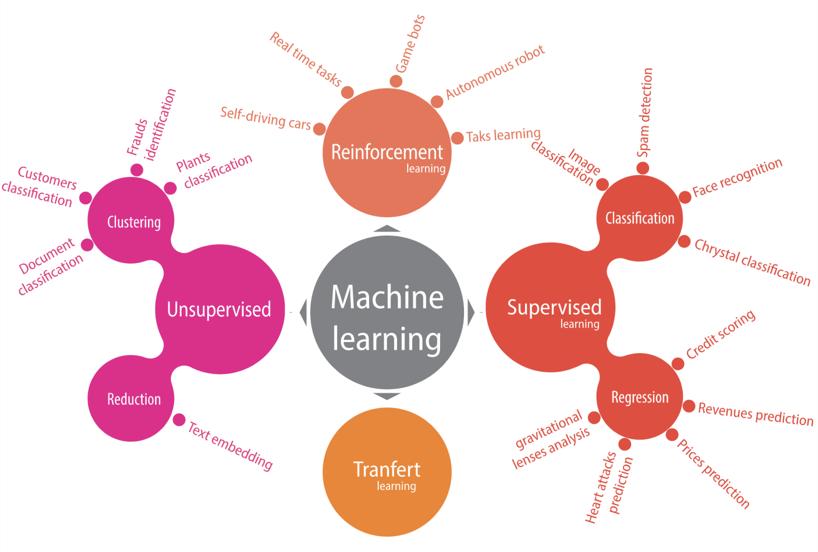
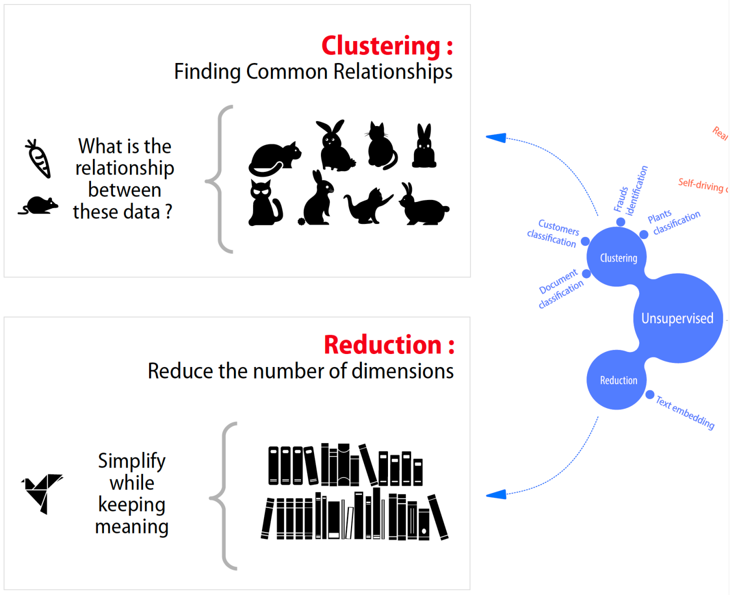
  Goal: learning by exploring the environment (e.g. games or autonomous vehicle)
- Transfer learning
  Goal: applying trained model to data of another type

Learning scenarios



source: fidle-cnrs

Unsupervised learning



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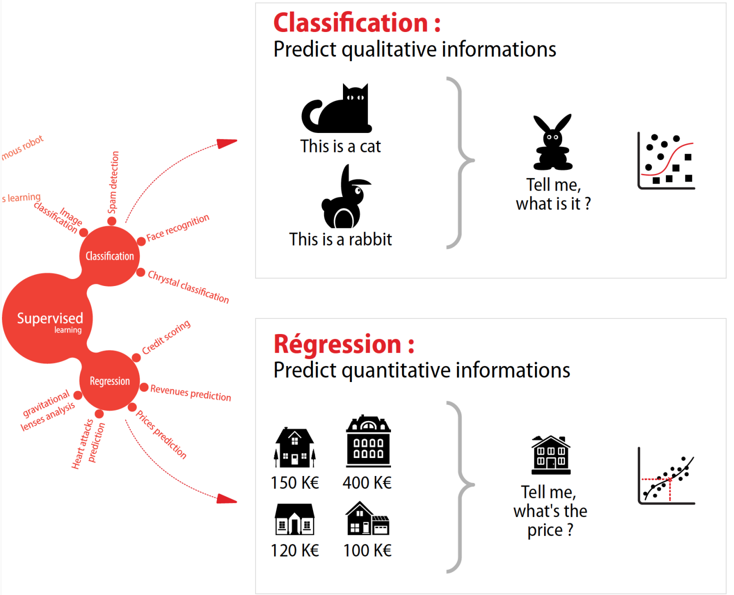
Supervised learning



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Main ML paradigms

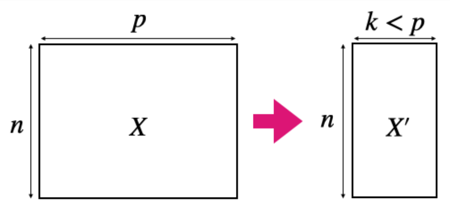
- Unsupervised learning
  - Dimension reduction
  - Clustering
  - Density estimation
  - Feature learning
- Supervised learning
  - Regression
  - Classification

Main ML paradigms

- Unsupervised learning
  - Dimension reduction: PCA
  - Clustering: k-means
  - Density estimation
  - Feature learning
- Supervised learning
  - Regression: linear (OLS), linear ridge regression
  - Classification: logistic regression, SVM

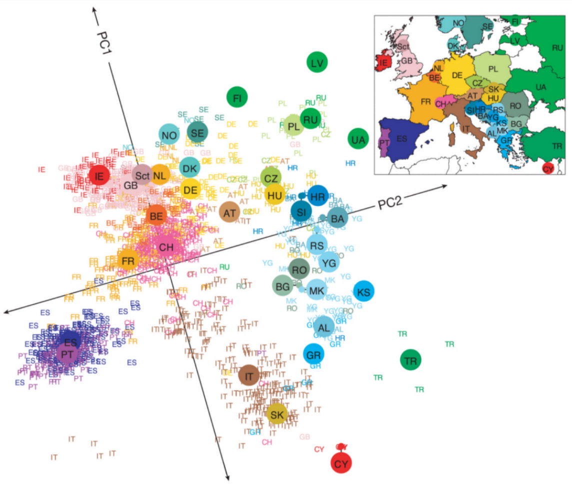
Contents

PCA: motivation



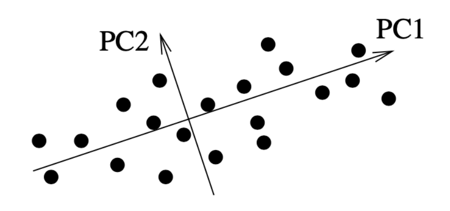
- Reduce the dimension without losing the variability in the data
- Visualization ($k = 2, 3$)
- Discover structure

Genetic data of 1387 Europeans: PCA ($k = 2$)



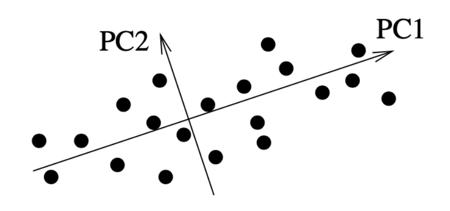
source: Novembre et al, 2008

PCA: definition



- The k-th principal component w_k:

PCA: definition



- The k-th principal component w_k:
  - is orthogonal to all previous components

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

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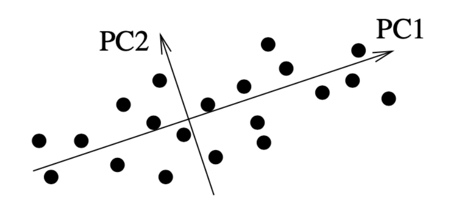

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$$\max_{\|w\|=1} w^\top X^\top X w = \max_{\|w\|=1} \|Xw\|^2$$

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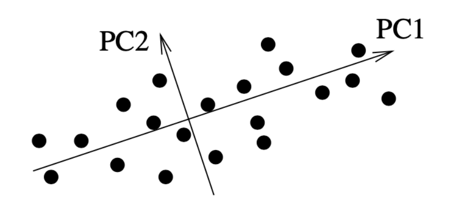

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($X^\top X$: empirical covariance of X (centered))

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

PCA: complexity

- Memory: store X and covariance matrix $X^\top X$: $\mathcal{O}(np)$, $\mathcal{O}(p^2)$
- Runtime:
  - Compute $X^\top X$: $\mathcal{O}(np^2)$
  - Compute k eigenvectors of $X^\top X$ with power methods: $\mathcal{O}(kp^2)$

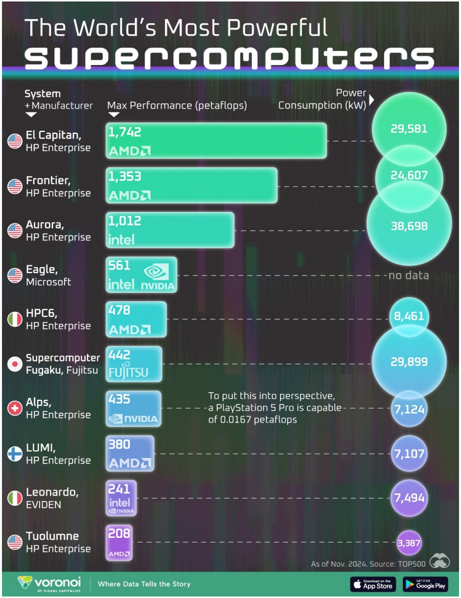
  Computing the covariance matrix is more expensive than computing its eigenvectors ($n > k$)!

Example

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

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

The most powerful computers



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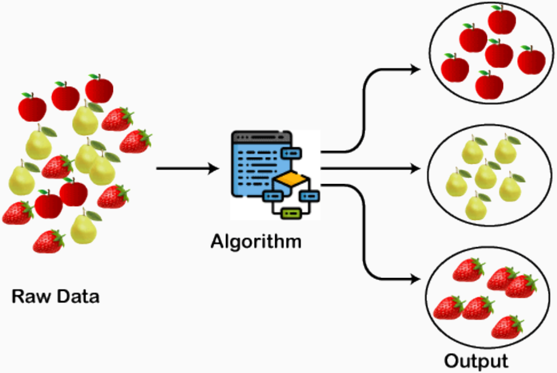
  World's fastest computer (Nov 2024):
  1,742 petaFLOPS (*Floating Point Operations per Second*) $\sim$ 1.7×10^{18} FLOPS
  $\rightarrow$ **68 days!**

Contents

Clustering: motivation



- Unsupervised learning
- Group samples
- Reduce dimensionality

k-means algorithm

- Dataset $\{\boldsymbol{x^1}, \ldots, \boldsymbol{x^n}\} \subset \mathbb{R}^p$

k-means algorithm

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$$\min_{c_i} \sum_{i=1}^{n} \|\boldsymbol{x^i} - \boldsymbol{\mu}_{c_i}\|^2,$$

where the $\boldsymbol{\mu}_j$, $j = 1, \ldots, k$, are the centroids

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

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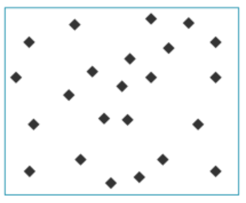

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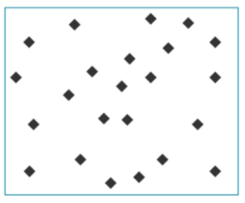

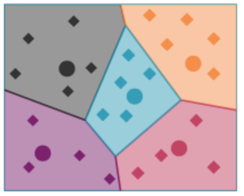

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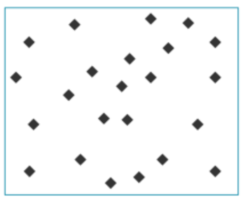

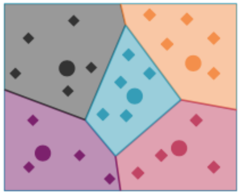

**Voronoi diagram*

Lloyd's algorithm (naïve k-means)

- Initialization:
  Randomly select k centroids $\boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_k$
- Iterations:
  1. Assignment step: assign the points to their nearest centroids

$$\forall i = 1, \ldots, n, \quad c_i \leftarrow \mathrm{argmin}_{c \in \{1,\ldots,k\}} \|\boldsymbol{x}^{\boldsymbol{i}} - \boldsymbol{\mu}_c\|$$

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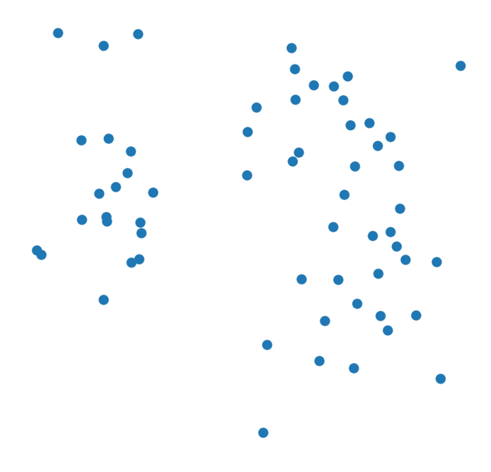
  2. Update step: update the centroids
  $$\forall i = 1, \ldots, k, \quad \boldsymbol{\mu}_i \leftarrow \frac{1}{|\{i : c_i = j\}|} \sum_{i:c_i=j} \boldsymbol{x}^{\boldsymbol{i}}$$

k-means example

$k = 3$



k-means example

- Select 3 centroids at random

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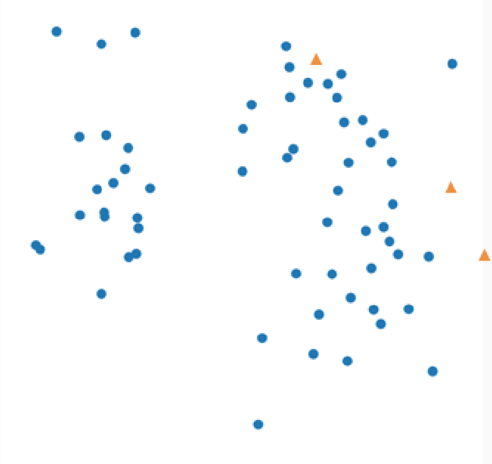
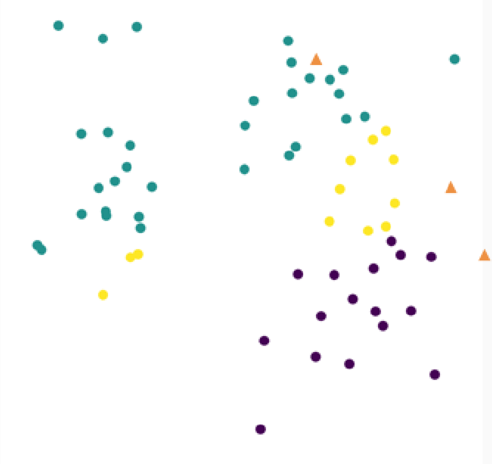


k-means example

- Assign each observation to the nearest centroid $k = 3$



k-means example

- Recompute centroids

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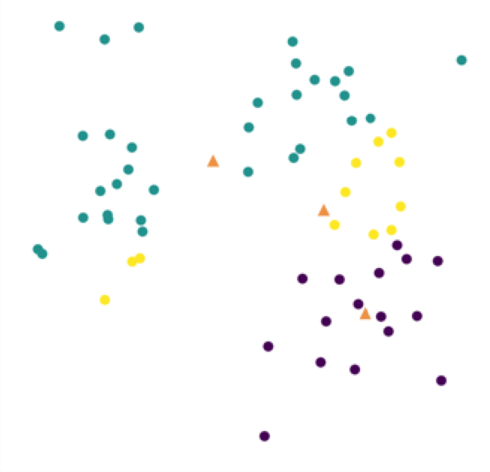
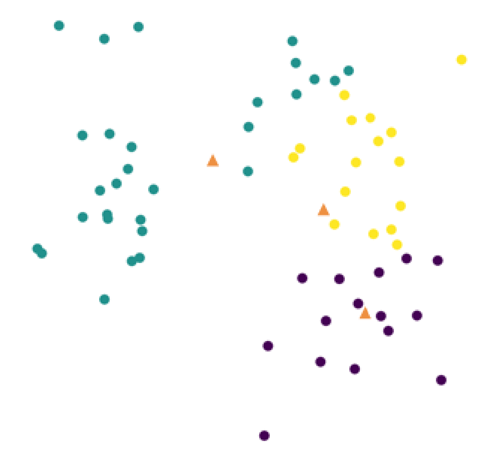


k-means example

- Re-assign each observation to the nearest centroid $k = 3$



k-means example

- Recompute centroids, and iterate process until convergence $\quad k = 3$

k-means complexity

- Runtime:

k-means complexity

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Compute $n \times k$ distances in $\mathbb{R}^p$: $\mathcal{O}(knp)$

k-means complexity

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    Sum n values in $\mathbb{R}^p$ for each centroid: $\mathcal{O}(knp)$

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

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    Sum n values in $\mathbb{R}^p$ for each centroid: $\mathcal{O}(knp)$
  - **Do T iterations**: $\mathcal{O}(kTnp)$
- Memory:
  - Store n cluster assignments and k centroids: $\mathcal{O}(n + kp)$

k-means complexity

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  - **Do T iterations**: $\mathcal{O}(kTnp)$
- Memory:
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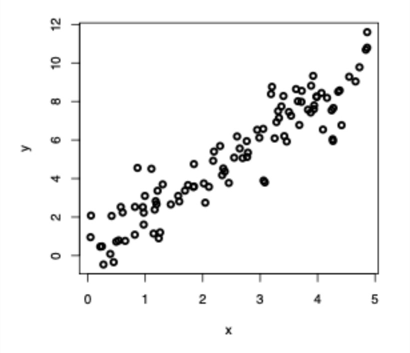
  - Store X: $\mathcal{O}(np)$

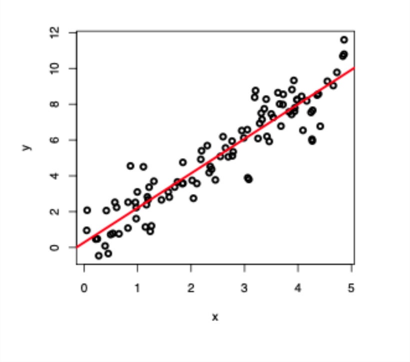
Contents

Linear regression: motivation



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

Linear regression: motivation



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$$\begin{aligned}\widehat{\boldsymbol{\beta}}^{\mathsf{OLS}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\ \mathsf{RSS}(\boldsymbol{\beta}) &= \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \sum_{i=1}^{n} (y^i - f_{\boldsymbol{\beta}}(\boldsymbol{x}^{\boldsymbol{i}}))^2 \\ &= \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \|\boldsymbol{y} - X\boldsymbol{\beta}\|^2\end{aligned}$$

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- Solution:

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

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

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$\rightarrow$ *unique and always exists !*

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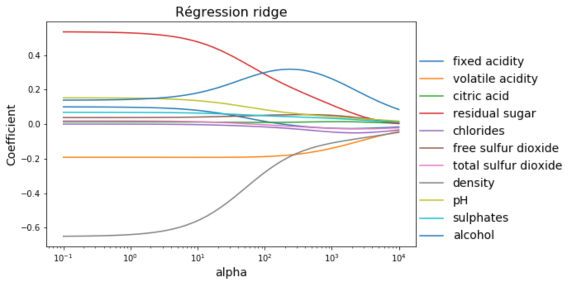
  $\rightarrow$ *unique and always exists !*
- Correlated features get similar weights
- Regularization reduces overfitting by penalizing larger weights, encouraging the model to prioritize simpler hypotheses

Ridge regression: limit cases

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

Corollary

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



Ridge regression: complexity

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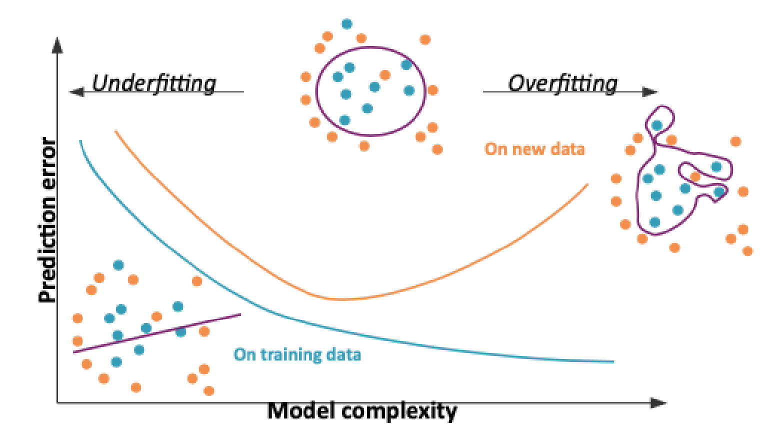
When $n \gg p$, computing $X^\top X + \lambda I$ is more expensive than inverting it!

Ridge regression: choice of λ



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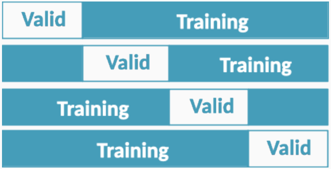

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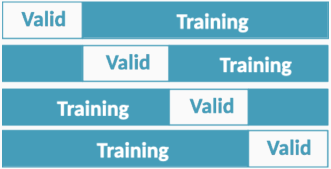

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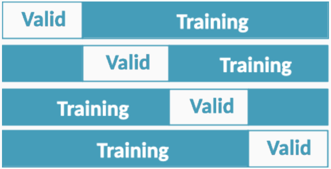

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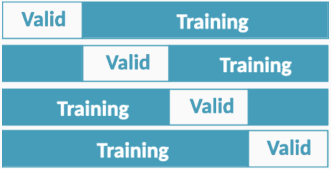

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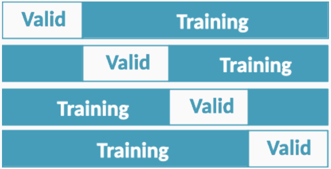

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- Multiplies complexity by KM!

Linear regression generalization: ℓ_2-regularized learning

- Generalization of the ridge regression to any loss:

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

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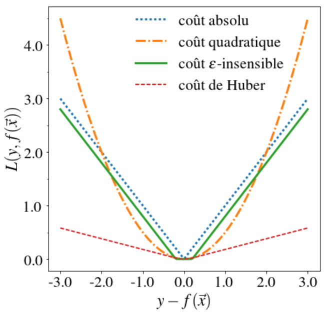
Loss examples

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

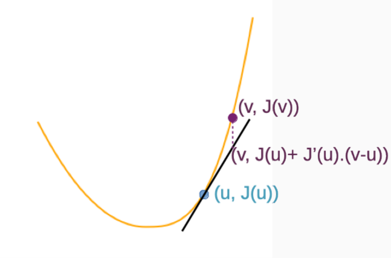


Numerical solution: gradient descent

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

- If we assume that the loss is differentiable, then

$$J(v) \geq J(u) + \nabla J(u)^\top (v - u)$$



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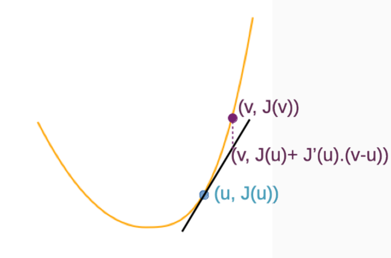
- $\nabla J(u) = 0 \Leftrightarrow u$ minimizes J



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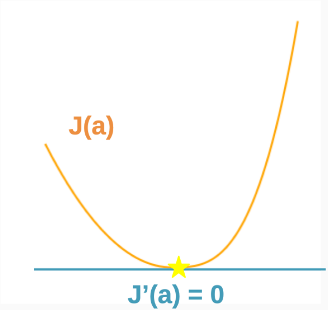

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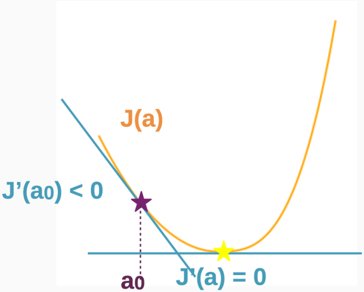

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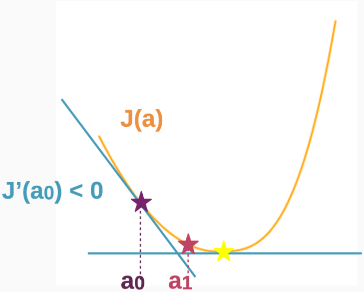

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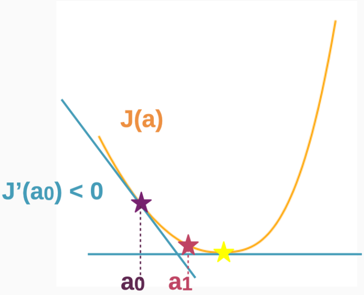

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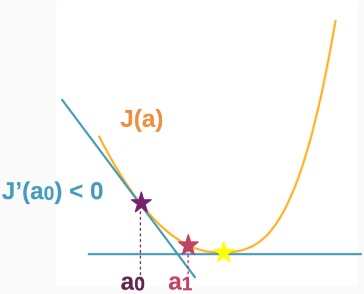

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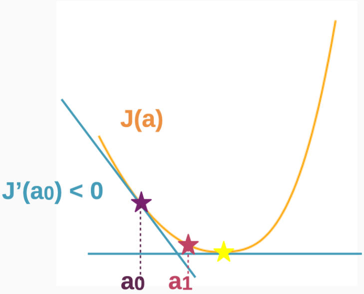

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- if α is too small $\rightarrow$ the algorithm is very slow
- if α is too big $\rightarrow$ a might oscillate around the minimum

Numerical solution: gradient descent

When to use gradient descent:

- Computing the analytical solution is too time-intensive (e.g., Ridge regression)
- Analytical solution for $\nabla J(a) = 0$ does not exist

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NB!

If J is not convex, we are not guaranteed to find a <u>global</u> minimum

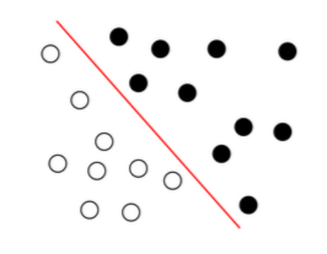
(we may need multiple restarts)

Contents

Classification: motivation

- Predict data labels (categories)
- There can be 2 or more (sometimes many) labels

Classification: linear models



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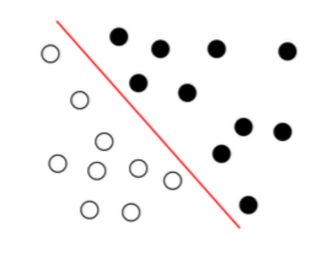

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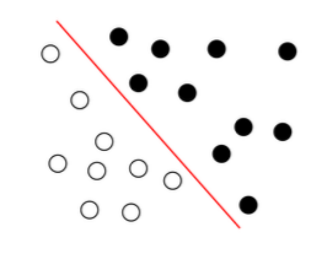

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$$f_{\boldsymbol{\beta}}(\boldsymbol{x}) = \boldsymbol{\beta}^\top \boldsymbol{x}$$
- Prediction for a new sample $\boldsymbol{x} \in \mathbb{R}^p$:
$$\begin{cases} +1 & \text{if } f_{\boldsymbol{\beta}}(\boldsymbol{x}) > 0\,, \\ -1 & \text{otherwise.} \end{cases}$$

Classification: the $0/1$ loss

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

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

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- Model is then tempting to learn $f_{\boldsymbol{\beta}}(\boldsymbol{x}) = \boldsymbol{\beta}^\top \boldsymbol{x}$ by solving:

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- However:
  - The problem is non-smooth, and typically NP-hard to solve
  - The regularization has no effect since the $0/1$ loss is invariant to scaling of $\boldsymbol{\beta}$

Classification: logistic loss

- Alternative approach:
  to define a probabilistic model of y parametrized by $f(\boldsymbol{x})$, e.g.:

$$\forall y \in \{-1, 1\}, \quad \mathbb{P}(y \,|\, f(\boldsymbol{x})) = \frac{1}{1 + e^{-y f(\boldsymbol{x})}} = \sigma(y f(\boldsymbol{x}))$$

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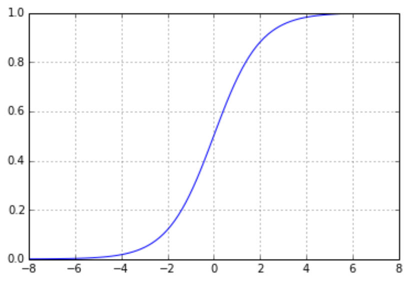

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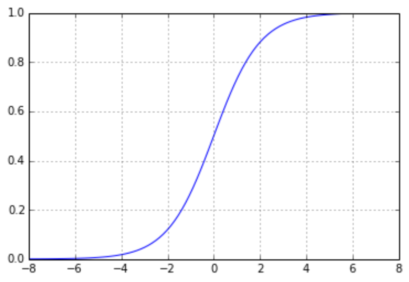

- The logistic loss is the negative conditional likelihood:

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

Classification: Ridge logistic regression

- *Cessie and Van Houwelingen, Ridge estimators in logistic regression, 1992*

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

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- Can be interpreted as a regularized conditional maximum likelihood estimator
- No analytical solution, but smooth convex optimization problem that can be solved numerically

Newton-Raphson iterations

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- Gradient descent:

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  where α is not constant
- Assume J is twice differentiable
  - Second-order Taylor's expansion:

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Newton-Raphson iterations

- Numerical method to minimize convex and differentiable J
- Gradient descent:

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  where α is not constant
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  - Take $\alpha = (\nabla^2 J(u_{t-1}))^{-1}$ in the gradient step

Solving ridge logistic regression

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

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- Solve with Newton-Raphson iterations

$$\begin{aligned}
\nabla_{\boldsymbol{\beta}} J(\boldsymbol{\beta}) &= -\frac{1}{n} \sum_{i=1}^{n} \frac{y^i \boldsymbol{x^i}}{1 + e^{y^i \boldsymbol{\beta}^\top \boldsymbol{x^i}}} + 2\lambda \boldsymbol{\beta} \\
&= -\frac{1}{n} \sum_{i=1}^{n} y^i [1 - \mathbb{P}_{\boldsymbol{\beta}}(y^i \,|\, \boldsymbol{x^i})] \boldsymbol{x^i} + 2\lambda \boldsymbol{\beta} \\
\nabla^2_{\boldsymbol{\beta}} J(\boldsymbol{\beta}) &= \frac{1}{n} \sum_{i=1}^{n} \frac{\boldsymbol{x^i} \boldsymbol{x}^{i\top} e^{y^i \boldsymbol{\beta}^\top \boldsymbol{x^i}}}{(1 + e^{y^i \boldsymbol{\beta}^\top \boldsymbol{x^i}})^2} + 2\lambda I \\
&= \frac{1}{n} \sum_{i=1}^{n} \mathbb{P}_{\boldsymbol{\beta}}(1 \,|\, \boldsymbol{x^i})(1 - \mathbb{P}_{\boldsymbol{\beta}}(1 \,|\, \boldsymbol{x^i})) \boldsymbol{x^i} \boldsymbol{x}^{i\top} + 2\lambda I
\end{aligned}$$

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$$\boldsymbol{\beta}_t \leftarrow \boldsymbol{\beta}_{t-1} - [\nabla^2_{\boldsymbol{\beta}} J(\boldsymbol{\beta}_{t-1})]^{-1} \nabla_{\boldsymbol{\beta}} J(\boldsymbol{\beta}_{t-1}) \,.$$

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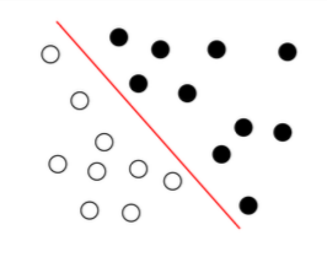
- Time complexity $\mathcal{O}(T(np^2 + p^3))$

Large-margin classifiers



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

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

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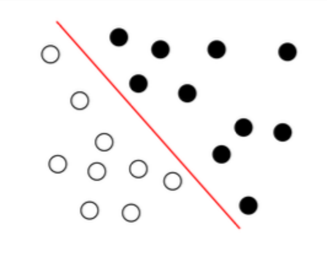

- For any $f : \mathbb{R}^p \to \mathbb{R}$, the margin of f on an $(\boldsymbol{x}, y)$ pair is

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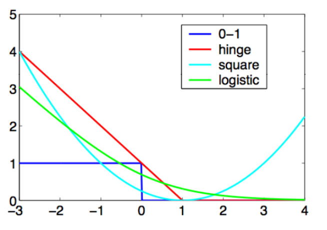
- Large-margin classifiers: maximize $y f(\boldsymbol{x})$:

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

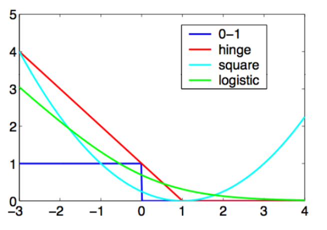
for a convex, non-increasing function $\phi : \mathbb{R} \to \mathbb{R}+$

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}

How to choose ϕ?



- Computation
  - convex $\phi \implies$ need to solve a convex optimization problem
  - Good choice of ϕ may allow fast optimization
- Theory
  - Most ϕ lead to consistent estimators
  - Some may be more efficient than others

Linear SVM

- *Boser, Guyon, and Vapnik, A training algorithm for optimal margin classifiers, 1992*

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

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- Primal problem is convex, but non-smooth
- Equivalent to Dual problem

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

$$\text{such that} \quad 0 \leq y^i \alpha_i \leq \frac{1}{2\lambda} \text{ for } i = 1, \ldots, n \text{ and } \sum_{i=1}^{n} \alpha_i y^i = 0.$$

Linear SVM

- Solution: $\boldsymbol{\beta}^* = \sum_{j=1}^{n} \alpha_j y^j \boldsymbol{x}^{\boldsymbol{j}} \qquad f_{\boldsymbol{\beta}^*}(\boldsymbol{x}) = \boldsymbol{\beta}^{*\top} \boldsymbol{x} = \sum_{j=1}^{n} \alpha_j y^j \boldsymbol{x}^{\boldsymbol{j}\top} \boldsymbol{x}$

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Complexity (training)

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Complexity (training)

- Primal: $\mathcal{O}(np^2 + p^3)$

Linear SVM

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Complexity (predicting)

- Primal: $\mathcal{O}(p)$

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Complexity (training)

- Primal: $\mathcal{O}(np^2 + p^3)$
- Dual: $\mathcal{O}(n^3 + pn^2)$

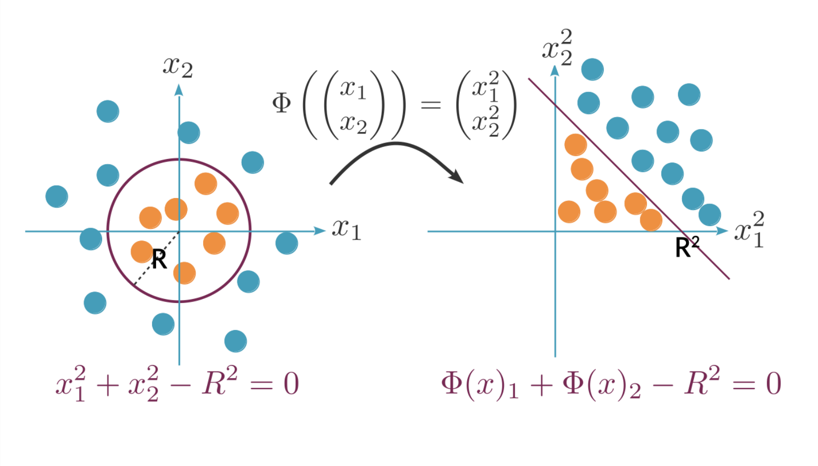
Complexity (predicting)

- Primal: $\mathcal{O}(p)$
- Dual: $\mathcal{O}(np)$

Contents

Kernel methods: motivation

Kernel methods: non-linear mapping



Kernel SVM

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

- **We have to use the dual form:**

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

$$\max_{\alpha \in \mathbb{R}^n} 2 \sum_{i=1}^{n} \alpha_i - \sum_{j,k=1}^{n} \alpha_j \alpha_k y^j y^k \langle \phi(\boldsymbol{x^j}), \phi(\boldsymbol{x^k}) \rangle_{\mathcal{H}}$$

- **Kernel k:**

$$k : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$$
$$(x, x') \mapsto k(x, x') = \langle \phi(x), \phi(x') \rangle$$

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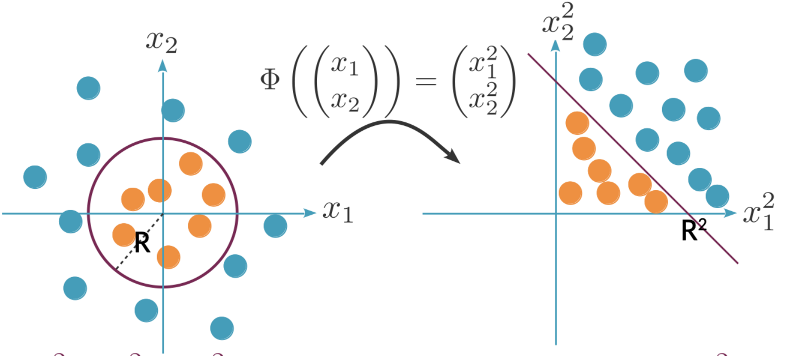
- **Kernels:**

$$\begin{aligned}
\text{Linear} \quad & k(\boldsymbol{x}, \boldsymbol{x'}) = \boldsymbol{x}^\top \boldsymbol{x'} \\
\text{Polynomial} \quad & k(\boldsymbol{x}, \boldsymbol{x'}) = (\boldsymbol{x}^\top \boldsymbol{x'} + c)^d \\
\text{Gaussian} \quad & k(\boldsymbol{x}, \boldsymbol{x'}) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x'}\|^2}{2\sigma^2}\right) \\
\text{Min/max} \quad & k(\boldsymbol{x}, \boldsymbol{x'}) = \sum_{j=1}^{p} \frac{\min(|x_j|, |x'_j|)}{\max(|x_j|, |x'_j|)}
\end{aligned}$$

Non-linear mapping to a feature space



$$x_1^2 + x_2^2 - R^2 = 0 \qquad \Phi(x)_1 + \Phi(x)_2 - R^2 = 0$$

$$K(\boldsymbol{x}, \boldsymbol{x}') = \left\langle \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \begin{pmatrix} {x_1'}^2 \\ {x_2'}^2 \end{pmatrix} \right\rangle = x_1^2 {x_1'}^2 + x_2^2 {x_2'}^2$$ [1]

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Summary

Method	Memory	Training time	Test time
PCA	$\mathcal{O}(p^2)$	$\mathcal{O}(np^2)$	$\mathcal{O}(p)$
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Things to worry about:

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- Training time: usually can take place offline
- Test time: prediction should be fast

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