Large Scale Machine Learning

Introduction to large-scale ML & optimization

March 2, 2026

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Acknowledgements

Slides inspired by:

- Adeline Fermanian
- Chloé-Agathe Azencott

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TECH

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

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

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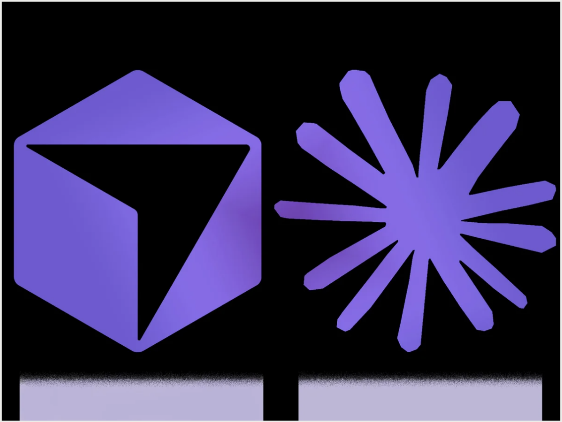
Machine learning is maybe the most sweltering thing in Silicon Valley at this moment. Particularly deep learning. The reason why it is so hot is on the grounds that it can assume control of numerous repetitive, thoughtless tasks. It'll improve doctors, and make lawyers better lawyers. What's more, it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

NEWS | AI

Was 2025 Really the Year of AI Agents? › Agents deliver gains for some engineers but give others pause

BY MATTHEW S. SMITH | 29 JAN 2026 | 5 MIN READ

Matthew S. Smith is a contributing editor for IEEE Spectrum and the former lead reviews editor at Digital Trends.



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TAGS

AI-AGENTS | AI-TOOLS | SOFTWARE-ENGINEERS | AGENTIC-AI

On 5 January 2025, OpenAI CEO Sam Altman outlined his vision for 2025 in a post on his personal blog. In it, Altman proclaimed that "in 2025, we may see the first AI agents 'join the workforce' and materially change the output of companies." His remarks set the tenor for the AI industry through 2025.

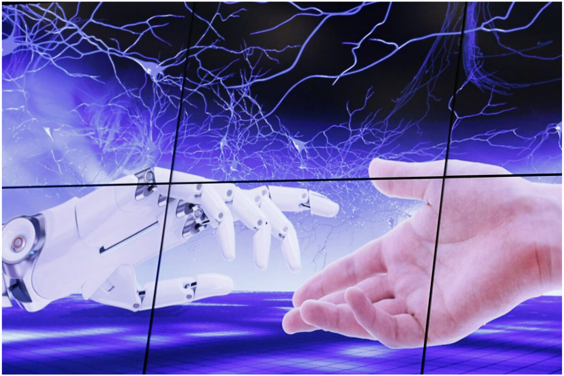
But did AI agents actually join the workforce in 2025? The answer is yes, absolutely—or no, not at all. It depends on who you ask.

Artificial Intelligencer: Why AI's math gold wins matter

By **Krystal Hu**

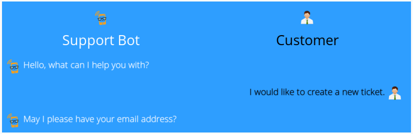
July 25, 2025 5:03 PM GMT+2 · Updated July 25, 2025

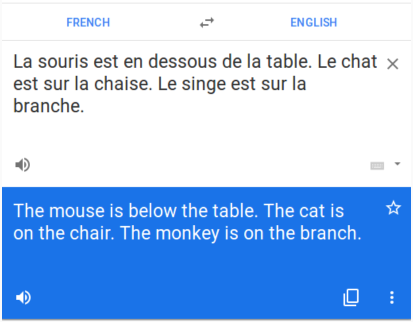
Aa



Perception

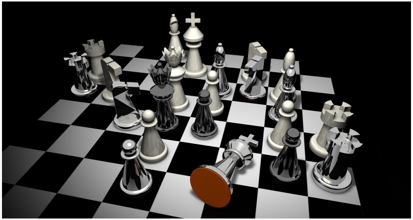
Communication

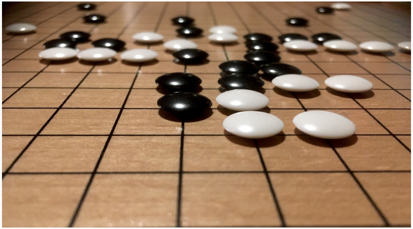




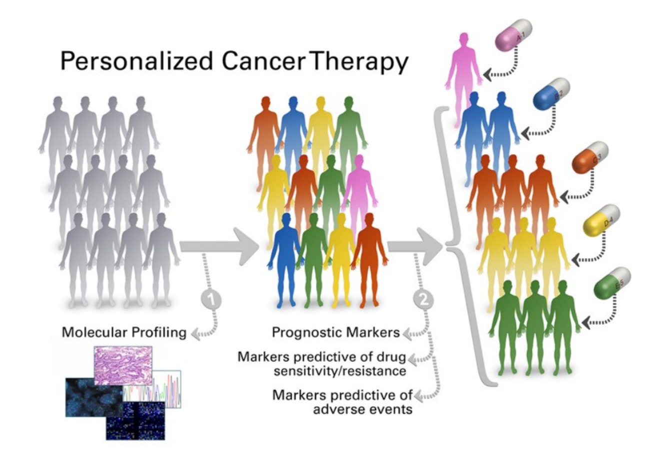
Mobility

Reasoning



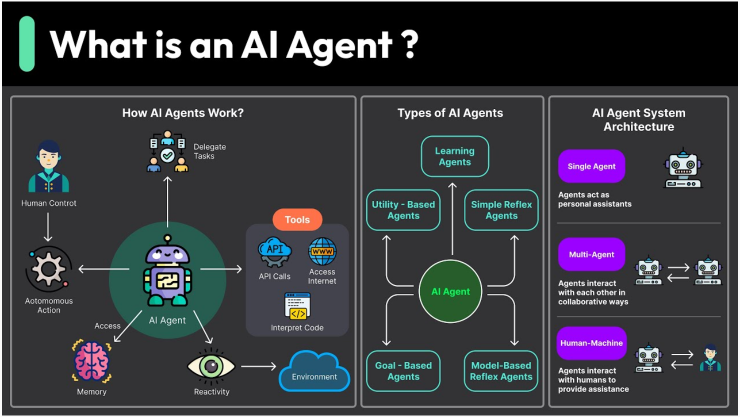


Health



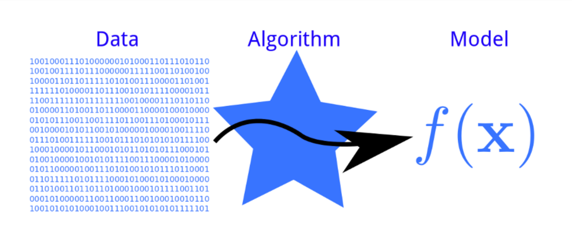
https://pct.mdanderson.org

AI Agent



What is an AI Agent ?
How AI Agents Work?
Human Controt
Delegate Tasks
Tools
API Calls
Access Internet
Interpret Code
Aotomomous Action
AI Agent
Access
Memory
Reactivity
Environment
Types of AI Agents
Learning Agents
Utility - Based Agents
Simple Reflex Agents
AI Agent
Goal - Based Agents
Model-Based Reflex Agents
AI Agent System Architecture
Single Agent
Agents act as personal assistants
Multi-Agent
Agents interact with each other in collaborative ways
Human-Machine
Agents interact with humans to provide assistance

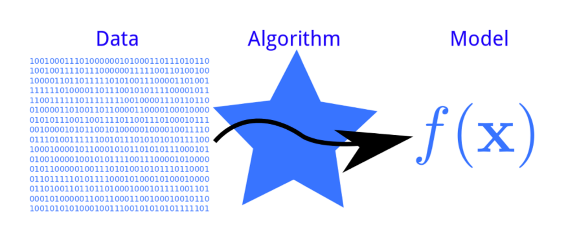
Learning from data



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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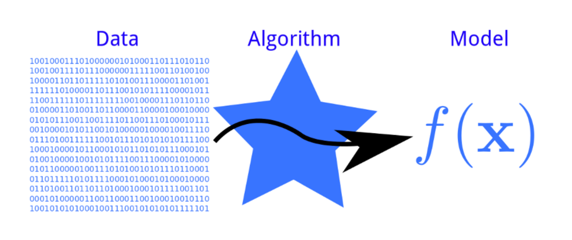

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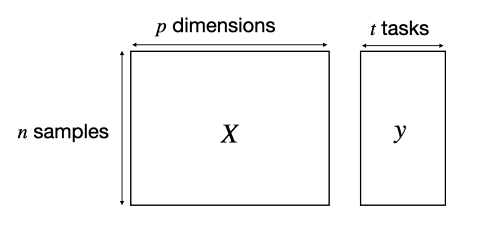
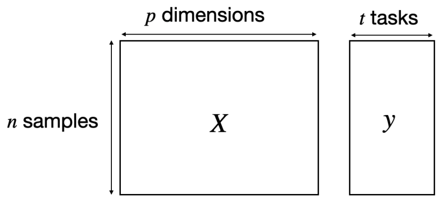
- Given: examples (training data)
  Goal: predict on new samples, or discover patterns in data
- Statistics + optimization + computer science
- Training gets better with more training examples and more powerful computers

Large-Scale Machine Learning



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: $n = 14{\cdot}10^6$, $p = 60{\cdot}10^3$, $t = 22{\cdot}10^3$
- Shopping, e-marketing $n = \mathcal{O}(10^6)$, $p = \mathcal{O}(10^9)$, $t = \mathcal{O}(10^8)$
- Astronomy, GAFAMs, web... $n = \mathcal{O}(10^9)$, $p = \mathcal{O}(10^9)$, $t = \mathcal{O}(10^9)$

Objectives for this lecture

1. Review several standard ML methods

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2. Discuss complexity of these methods

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1. Review several standard ML methods
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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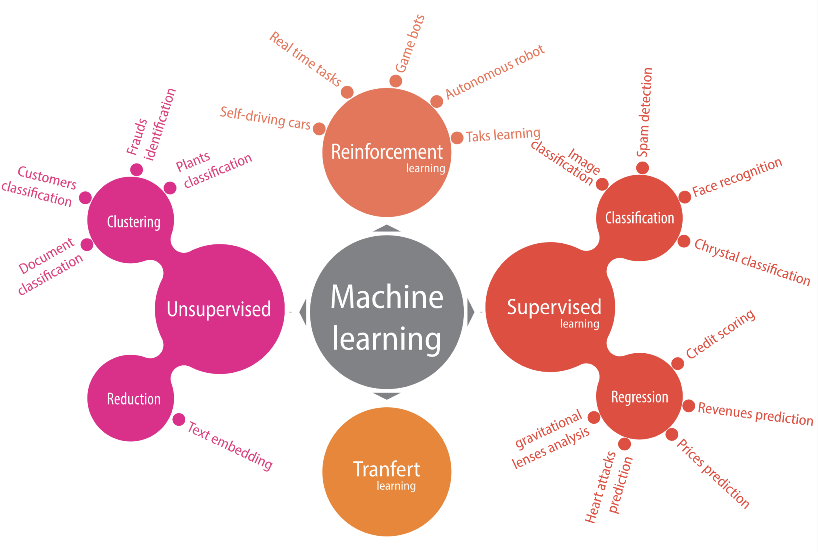
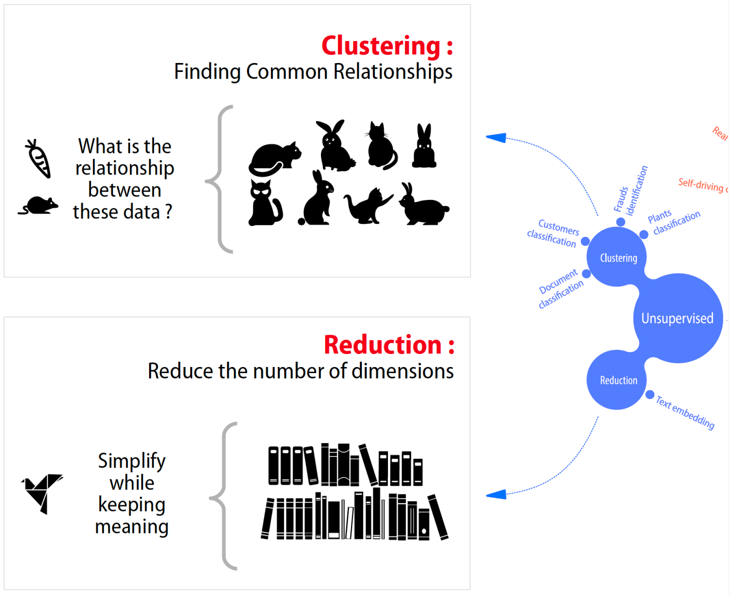
- Transfer learning
  Goal: applying trained model to data of another type

Learning scenarios

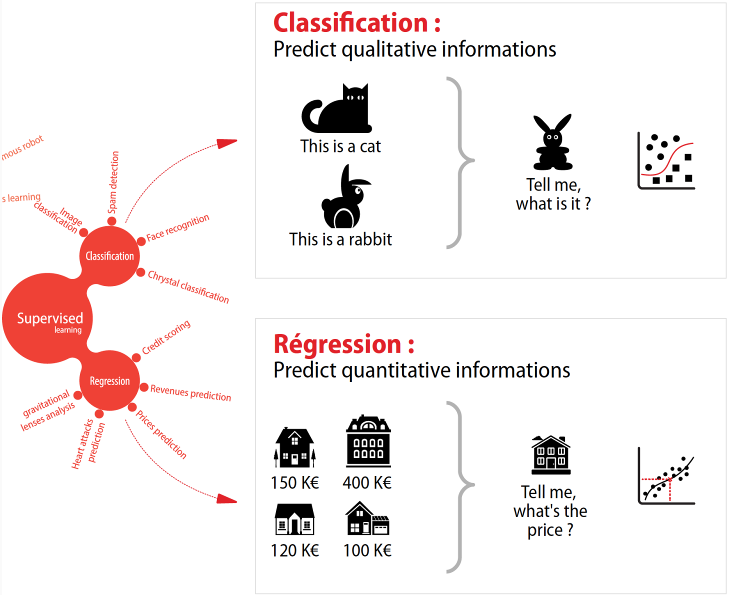


source: fidle-cnrs

Unsupervised learning



Supervised learning



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Main ML paradigms

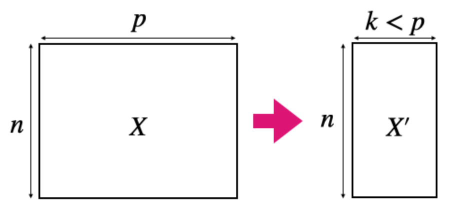
- Unsupervised learning
  - Dimension reduction
  - Clustering
  - Density estimation
  - Feature learning
- Supervised learning
  - Regression
  - Classification

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

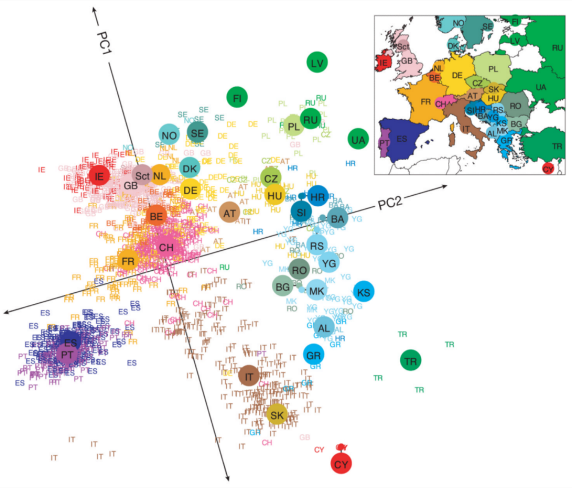
PCA: motivation



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

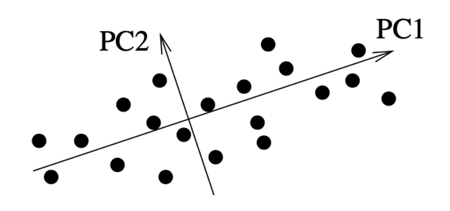
PCA: motivation example

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



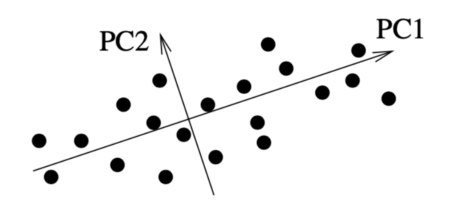
source: Novembre et al, 2008

PCA: definition



- $\forall k$, the k-th principal component w_k:

PCA: definition



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  - is orthogonal to all previous components

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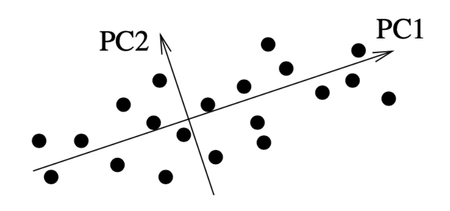

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($X^\top X$: empirical covariance of X (centered))

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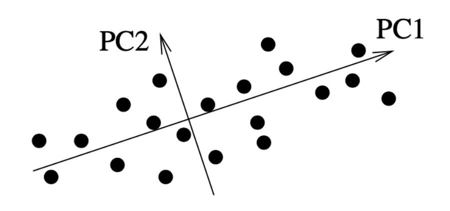

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($X^\top X$: empirical covariance of X (centered))

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

PCA: complexity

- Memory: store X and covariance matrix $X^\top X$: $\mathcal{O}(np)$, $\mathcal{O}(p^2)$

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  - Compute $X^\top X$: $\mathcal{O}(np^2)$
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Computing the covariance matrix is more expensive than computing its eigenvectors ($n > k$)!

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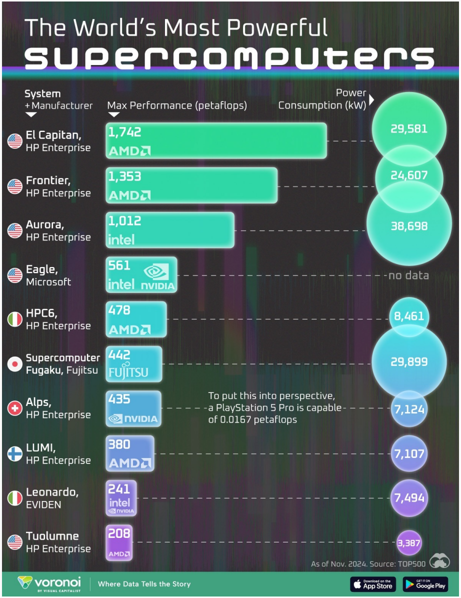
Example

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

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

The most powerful computers



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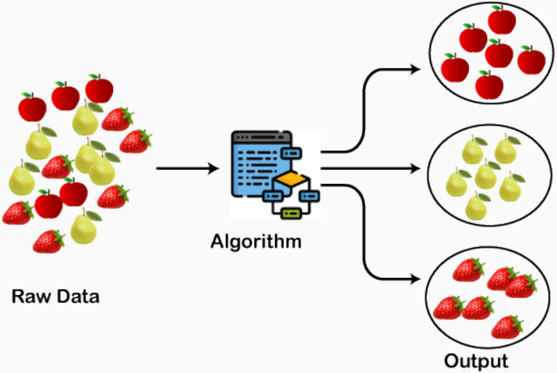
  World's fastest computer (Nov 2024):
  1,742 petaFLOPS (*Floating Point Operations per Second*) $\sim$
  1.7×10^{18} FLOPS
  $\rightarrow$ **68 days!**

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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- Find a cluster assignment $c_i \in \{1, \dots, k\}$ for all $i = 1, \dots, n$ that minimizes the intra-cluster variance:

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

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

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

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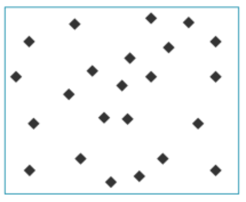

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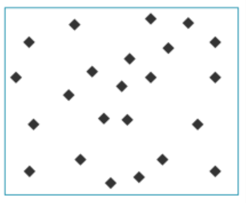

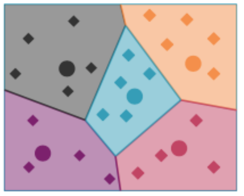

*Voronoi diagram

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

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

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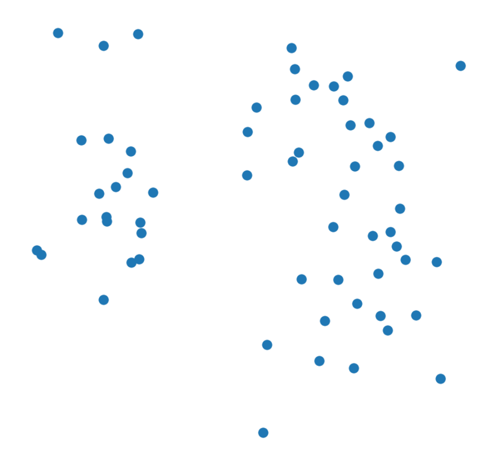
  2. Update step: update the centroids
  $$\forall i = 1, \dots, k, \quad \boldsymbol{\mu}_i \leftarrow \frac{1}{|\{i : c_i = j\}|} \sum_{i:c_i=j} \boldsymbol{x}^{\boldsymbol{i}}$$

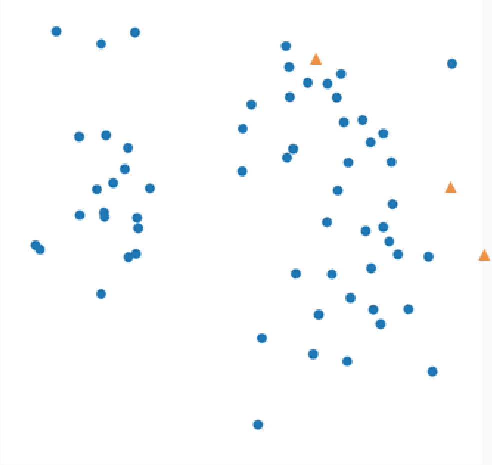
k-means example

$k = 3$



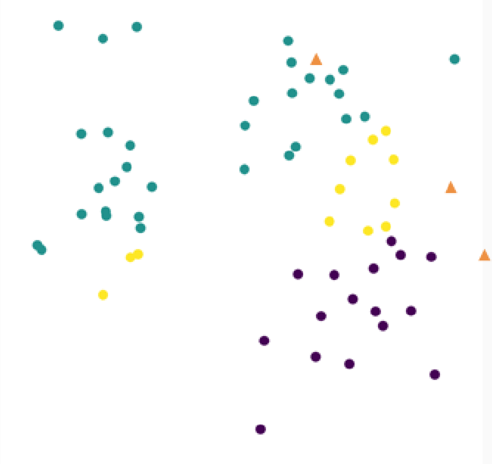
k-means example

▷ Select 3 centroids at random $k = 3$



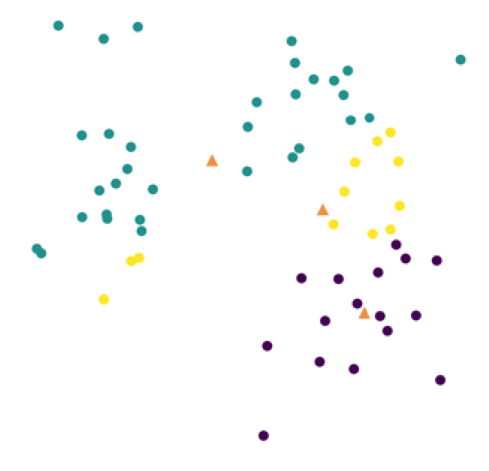
k-means example

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



k-means example

- Recompute centroids $k = 3$



k-means example

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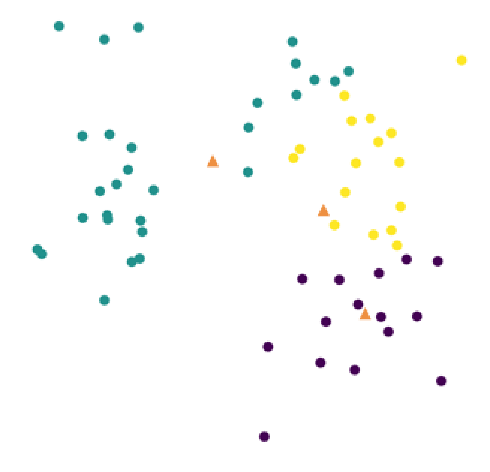

k-means example

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

k-means complexity

- Runtime:

k-means complexity

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k-means complexity

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  - **Do T iterations**: $\mathcal{O}(kTnp)$
  - **NB!** We may need to try different numbers of clusters k

k-means complexity

- Runtime:
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k-means complexity

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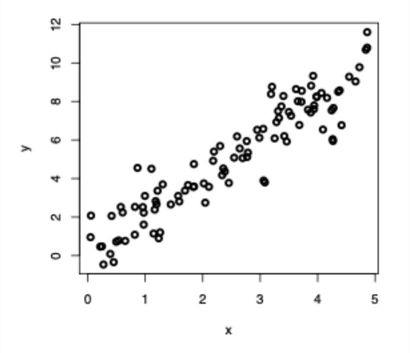
  - Store X: $\mathcal{O}(np)$

Contents

Linear regression: motivation



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

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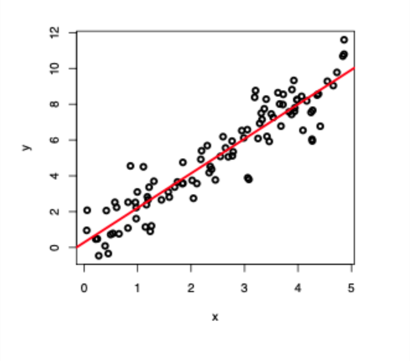

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- Quality of fit is measured as a Residual Sum of Squares (RSS):

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- Solution:

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

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

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  $\rightarrow$ *unique and always exists !*

- Correlated features get similar weights

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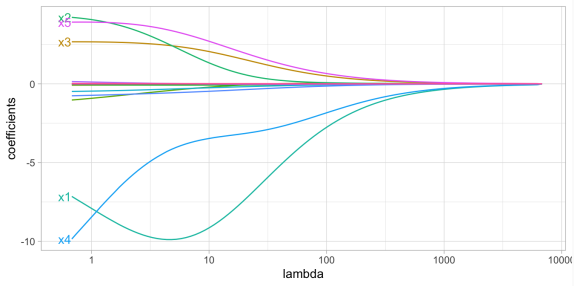
- Correlated features get similar weights
- Regularization reduces overfitting by penalizing larger weights, encouraging the model to prioritize simpler hypotheses

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).



from "Hands-on machine learning with R"

Ridge regression: complexity

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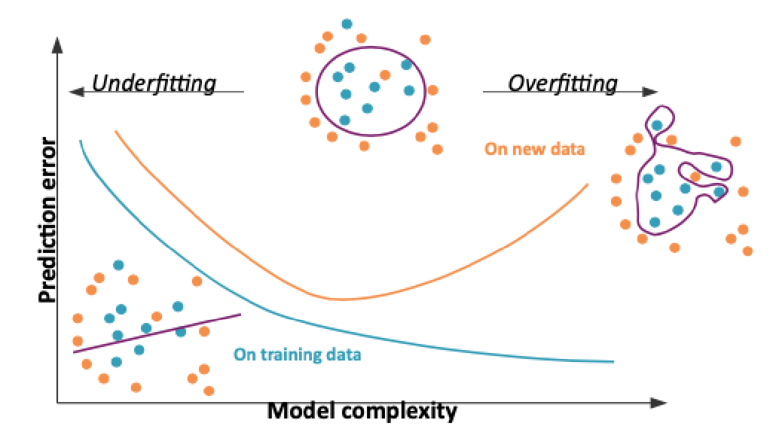
When $n \gg p$, computing $X^\top X + \lambda I$ is more expensive than inverting it!

Ridge regression: choice of λ



Ridge regression: choice of λ

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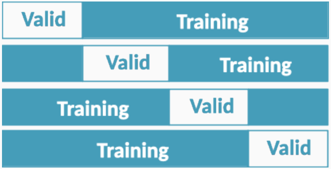
  - Split the training set (of size n) into K equally-sized chunks



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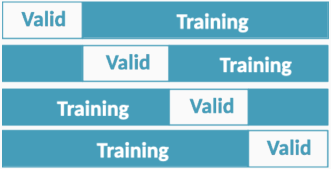

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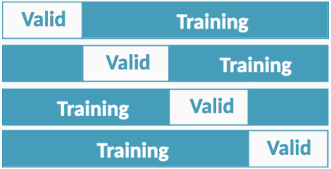

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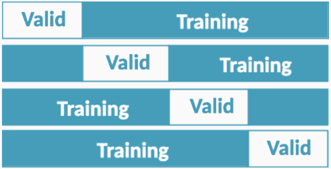

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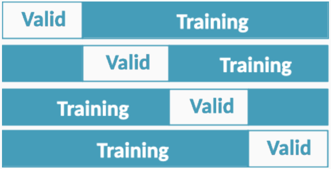

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- Multiplies complexity by KM!

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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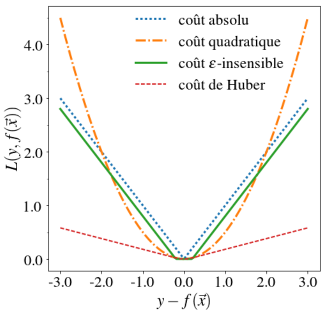
Loss examples

- 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

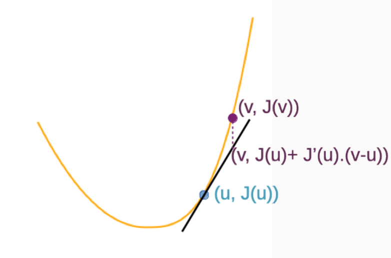


Numerical solution: gradient descent

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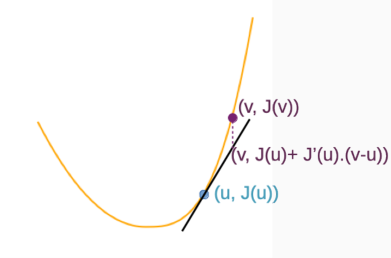
- $\nabla J(u) = 0 \Leftrightarrow u$ minimizes J



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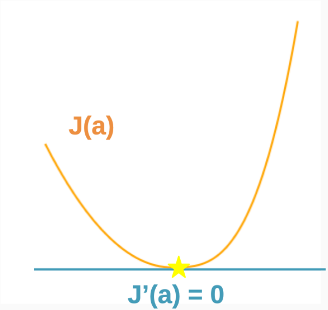

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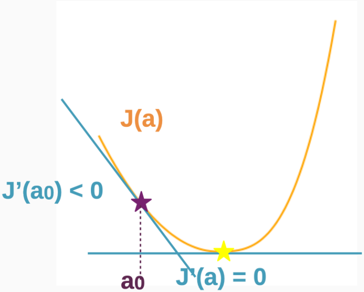

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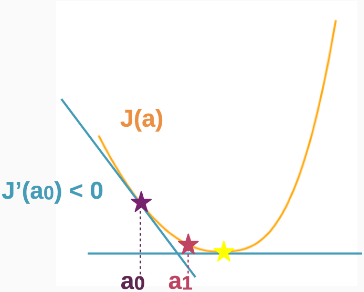

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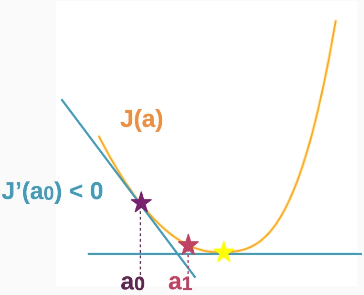

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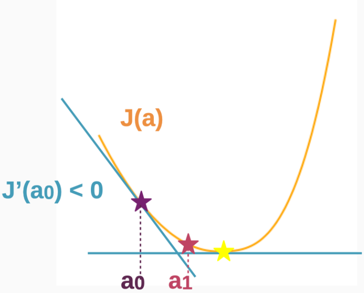

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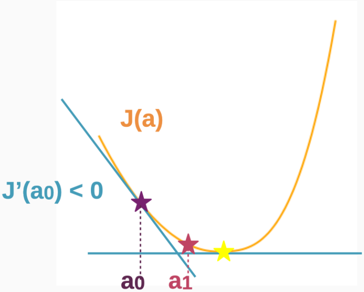

α – learning rate

- 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-consuming (e.g., Ridge regression)
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NB!

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

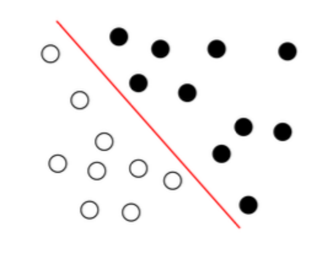
(we may need multiple restarts)

Contents

Classification: motivation

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

Classification: linear models



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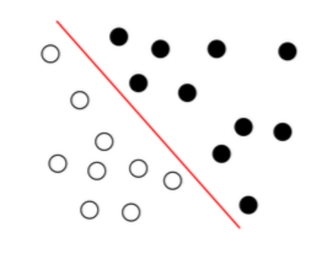

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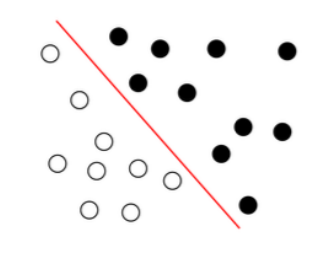

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- Fit a linear function

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

- 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:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell_{0/1}(f_{\boldsymbol{\beta}}(\boldsymbol{x}^{\boldsymbol{i}}), y^i)}_{\text{misclassification rate}} + \underbrace{\lambda \|\boldsymbol{\beta}\|^2}_{\text{regularization}}$$

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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.:

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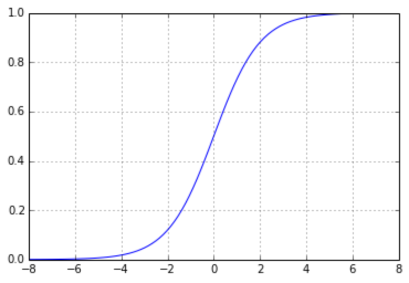

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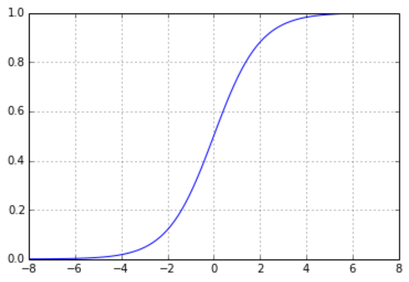

- The logistic loss is the negative conditional likelihood:

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

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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  - Take $\alpha = (\nabla^2 J(u_{t-1}))^{-1}$ in the gradient step

Solving ridge logistic regression

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

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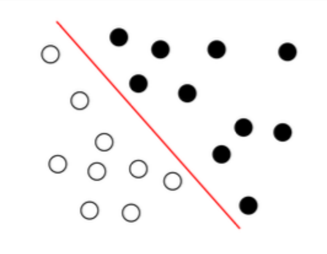
- Time complexity $\mathcal{O}(T(np^2 + p^3))$

Large-margin classifiers



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

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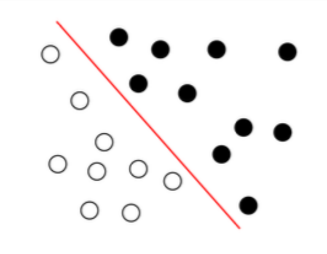

- For any $f : \mathbb{R}^p \to \mathbb{R}$, the margin of f on an $(\boldsymbol{x}, y)$ pair is

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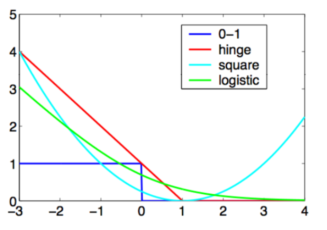
- Large-margin classifiers: maximize $y f(\boldsymbol{x})$:

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

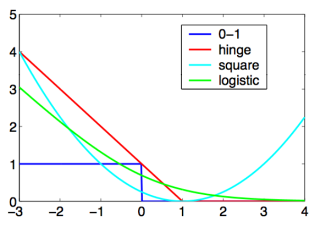
for a convex, non-increasing function $\phi : \mathbb{R} \to \mathbb{R}+$

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
    (accuracy increases when there is more data)
  - Some may be more efficient than others

Linear SVM

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

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

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

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

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

Linear SVM

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

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Complexity (training)

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

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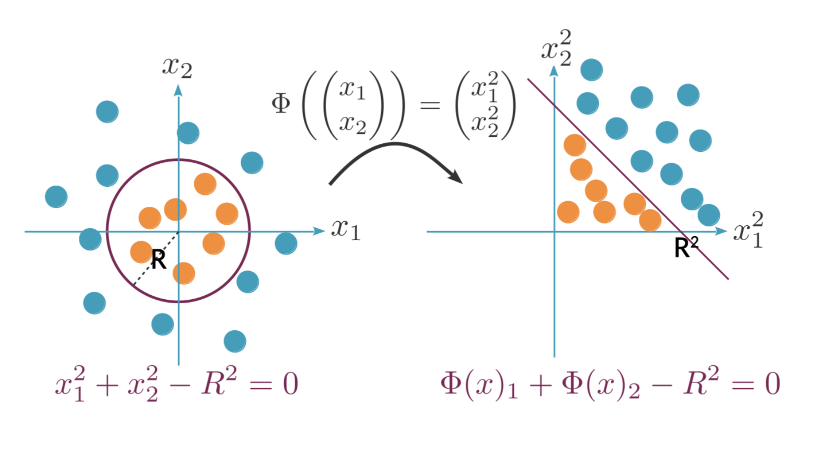
Contents

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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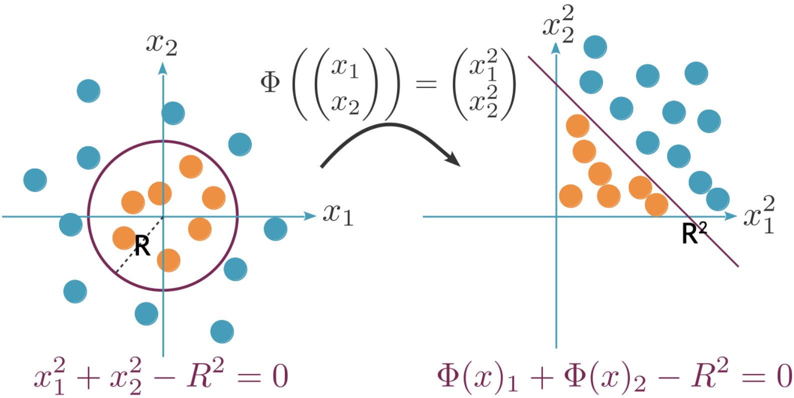
- **Kernels:**

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

Non-linear mapping to a feature space



$$K(\boldsymbol{x}, \boldsymbol{x}') = \left\langle \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}, \begin{pmatrix} {x'_1}^2 \\ {x'_2}^2 \end{pmatrix} \right\rangle = x_1^2 {x'_1}^2 + x_2^2 {x'_2}^2$$ [1]

Contents

Summary

Method	Memory	Training time	Test time
PCA	$\mathcal{O}(p^2)$	$\mathcal{O}(np^2)$	$\mathcal{O}(p)$
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Ridge regression	$\mathcal{O}(p^2)$	$\mathcal{O}(np^2 + p^3)$	$\mathcal{O}(p)$
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Things to worry about:

- Memory requirements
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Questions?