# Large-Scale Machine Learning 

Jean-Philippe Vert

jean-philippe.vert@\{mines-paristech, curie,ens\}.fr

Together, let's beat cancer.

## Outline

(1) Introduction
(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning
- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4) Conclusion

## Acknowledgement

In the preparation of these slides I got inspiration and copied several slides from several sources:

- Sanjiv Kumar's "Large-scale machine learning" course: http://www.sanjivk.com/EECS6898/lectures.html
- Ala Al-Fuqaha's "Data mining" course: https://cs.wmich.edu/alfuqaha/summer14/cs6530/ lectures/SimilarityAnalysis.pdf
- Léon Bottou's "Large-scale machine learning revisited" conference https://bigdata2013.sciencesconf.org/conference/ bigdata2013/pages/bottou.pdf


## Outline

(1) Introduction
(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning
- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

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

| ■ GAURAV SANGWANI | 甲 0 | JAN 13, 2017, 12.51PM |
| :---: | :---: | :---: |



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



## Health

## Personalized CancerTherapy


https://pct.mdanderson.org

Reasoning


## A common process: learning from data

## Data

100100011101000000101000110111010110 100100111101110000001111100110100100 100001101101111101010011100001101001 111111010000110111001010111100001011 110011111101111111100100001110110110 010000110100110110000110000100010000 010101110011001111011001110100010111 001000010101100101000001000010011110 011101001111110010111010101010111100 100010000101100010101101010111000101 010010000100101011110011100001010000 010110000010011101010010101110110001 011011111010111100010100010100010000 011010011011011010001000101111001101 000101000001100110001100100010010110 100101010100010011100101010101111101

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

- 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?

## d dimensions



## t tasks



- Iris dataset: $n=150, d=4, t=1$
- Cancer drug sensitivity: $n=1 k, d=1 M, t=100$
- Imagenet: $n=14 M, d=60 k+, t=22 k$
- Shopping, e-marketing $n=O(M), d=O(B), t=O(100 M)$
- Astronomy, GAFA, web... $n=O(B), d=O(B), t=O(B)$


## Today's goals

(1) Review a few standard ML techniques



(2) Introduce a few ideas and techniques to scale them to modern, big datasets


## Outline

(1) Introduction
(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning
- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## 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
- Classification: kNN, logistic regression, SVM
- Structured output classification
- Semi-supervised learning
- Reinforcement learning


## Outline

## (1) Introduction

(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: k-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning

4 Conclusion

## Motivation



- Dimension reduction
- Preprocessing (remove noise, keep signal)
- Visualization ( $k=2,3$ )
- Discover structure


## PCA definition



- Training set $\mathcal{S}=\left\{x_{1}, \ldots, x_{n}\right\} \subset \mathbb{R}^{d}$
- For $i=1, \ldots, k \leq d, P C_{i}$ is the linear projection onto the direction that captures the largest amount of variance and is orthogonal to the previous ones:

$$
u_{i} \in \underset{\|u\|=1, u \perp\left\{u_{1}, \ldots, u_{i-1}\right\}}{\operatorname{argmax}} \sum_{i=1}^{n}\left(x_{i}^{\top} u-\frac{1}{n} \sum_{j=1}^{n} x_{j}^{\top} u\right)^{2}
$$

## PCA solution



- Let $\tilde{X}$ be the centered $n \times d$ data matrix
- PCA solves, for $i=1, \ldots, k \leq d$ :

$$
u_{i} \in \underset{\|u\|=1, u \perp\left\{u_{1}, \ldots, u_{i-1}\right\}}{\operatorname{argmax}} u^{\top} \tilde{X}^{\top} \tilde{X} u
$$

- Solution: $u_{i}$ is the $i$-th eigenvector of $C=\tilde{X}^{\top} \tilde{X}$, the empirical covariance matrix


## PCA example

Iris dataset

> data(iris)
> head(iris, 3)
Sepal.Length Sepal.Width Petal.Length Petal.Width Species

| 1 | 5.1 | 3.5 | 1.4 | 0.2 | setosa |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 | setosa |
| 3 | 4.7 | 3.2 | 1.3 | 0.2 | setosa |
| $>m$ | <- princomp(log(iris[,1:4])) |  |  |  |  |

## PCA complexity

- Memory: store $X$ and $C: O\left(\max \left(n d, d^{2}\right)\right)$
- Compute C: $O\left(n d^{2}\right)$
- Compute $k$ eigenvectors of $C$ (power method): $O\left(k d^{2}\right)$

Computing $C$ is more expensive than computing its eigenvectors $(n>k)$ !
$n=1 B, d=100 M$
Store C: 40, 000TB
Compute C: $2 \times 10^{25}$ FLOPS $=20$ yottaFLOPS (about 300 years of the most powerful supercomputer in 2016)

## Outline

## (1) Introduction

(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: k-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning

4 Conclusion

## Motivation

Iris dataset


- Unsupervised learning
- Discover groups
- Reduce dimension


## Motivation

Iris k-means, $k=5$


- Unsupervised learning
- Discover groups
- Reduce dimension


## $k$-means definition

- Training set $\mathcal{S}=\left\{x_{1}, \ldots, x_{n}\right\} \subset \mathbb{R}^{d}$
- Given $k$, find $C=\left(C_{1}, \ldots, C_{n}\right) \in\{1, k\}^{n}$ that solves

$$
\min _{C} \sum_{i=1}^{n}\left\|x_{i}-\mu_{C_{i}}\right\|^{2}
$$

where is the barycentre of data in class $i$.

- This is an NP-hard problem. $k$-means finds an approximate solution by iterating
(1) Assignment step: fix $\mu$, optimize $C$

$$
\forall i=1, \ldots, n, \quad C_{i} \leftarrow \arg \min _{c \in\{1, \ldots, k\}}\left\|x_{i}-\mu_{g}\right\|
$$

(2) Update step

$$
\forall i=1, \ldots, k, \quad \mu_{i} \leftarrow \frac{1}{\left|C_{i}\right|} \sum_{j: C_{j}=i} x_{j}
$$

## $k$-means example

Iris dataset

> irisCluster <- kmeans(log(iris[, 1:4]), 3, nstart = 20)
> table(irisCluster\$cluster, iris\$Species)

|  | setosa | versicolor | virginica |
| ---: | ---: | ---: | ---: |
| 1 | 0 | 48 | 4 |
| 2 | 50 | 0 | 0 |
| 3 | 0 | 2 | 46 |

## $k$-means example

Iris $\mathbf{k}$-means, $\mathbf{k}=\mathbf{2}$

> irisCluster <- kmeans(log(iris[, 1:4]), 3, nstart = 20)
> table(irisCluster\$cluster, iris\$Species)

|  | setosa | versicolor | virginica |
| ---: | ---: | ---: | ---: |
| 1 | 0 | 48 | 4 |
| 2 | 50 | 0 | 0 |
| 3 | 0 | 2 | 46 |

## $k$-means example

Iris $\mathbf{k}$-means, $\mathbf{k}=\mathbf{3}$

> irisCluster <- kmeans(log(iris[, 1:4]), 3, nstart = 20)
> table(irisCluster\$cluster, iris\$Species)

|  | setosa | versicolor | virginica |
| ---: | ---: | ---: | ---: |
| 1 | 0 | 48 | 4 |
| 2 | 50 | 0 | 0 |
| 3 | 0 | 2 | 46 |

## $k$-means example

Iris $\mathbf{k}$-means, $\mathrm{k}=4$

> irisCluster <- kmeans(log(iris[, 1:4]), 3, nstart = 20)
> table(irisCluster\$cluster, iris\$Species)

|  | setosa | versicolor | virginica |
| ---: | ---: | ---: | ---: |
| 1 | 0 | 48 | 4 |
| 2 | 50 | 0 | 0 |
| 3 | 0 | 2 | 46 |

## $k$-means example

Iris $k$-means, $k=5$

> irisCluster <- kmeans(log(iris[, 1:4]), 3, nstart = 20)
> table(irisCluster\$cluster, iris\$Species)

|  | setosa | versicolor | virginica |
| ---: | ---: | ---: | ---: |
| 1 | 0 | 48 | 4 |
| 2 | 50 | 0 | 0 |
| 3 | 0 | 2 | 46 |

## k-means complexity

- Each update step: $O(n d)$
- Each assgnment step: $O(n d k)$


## Outline

## (1) Introduction

(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: k-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning

4 Conclusion

## Motivation



- Predict a continuous output from an input


## Motivation



- Predict a continuous output from an input


## Model

- Training set $\mathcal{S}=\left\{\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right)\right\} \subset \mathbb{R}^{d} \times \mathbb{R}$
- Fit a linear function:

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

- Goodness of fit measured by residual sum of squares:

$$
\operatorname{RSS}(\beta)=\sum_{i=1}^{n}\left(y_{i}-f_{\beta}\left(x_{i}\right)\right)^{2}
$$

- Ridge regression minimizes the regularized RSS:

$$
\min _{\beta} R S S(\beta)+\lambda \sum_{i=1}^{d} \beta_{i}^{2}
$$

- Solution (set gradient to 0 ):

$$
\hat{\beta}=\left(X^{\top} X+\lambda I\right)^{-1} X^{\top} Y
$$

## Ridge regression complexity

- Compute $X^{\top} X: O\left(n d^{2}\right)$
- Inverse $\left(X^{\top} X+\lambda I\right): O\left(d^{3}\right)$

Computing $X^{\top} X$ is more expensive than inverting it!

## Outline

## (1) Introduction

(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning

4 Conclusion

## Motivation



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


## Motivation



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


## Motivation



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


## Motivation



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


## k-nearest neigbors (kNN)


(Hastie et al. The elements of statistical learning. Springer, 2001.)

- Training set $\mathcal{S}=\left\{\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right)\right\} \subset \mathbb{R}^{d} \times\{-1,1\}$
- No training
- Given a new point $x \in \mathbb{R}^{d}$, predict the majority class among its $k$ nearest neighbors (take $k$ odd)


## kNN properties

Uniform Bayes consistency [Stone, 1977]

- Take $k=\sqrt{n}$ (for example)
- Let $P$ be any distribution over $(X, Y)$ pairs
- Assume training data are random pairs sampled i.i.d. according to $P$
- Then the $k$-NN classifier $\hat{f}_{n}$ satisfies almost surely:

$$
\lim _{n \rightarrow+\infty} P(\hat{f}(X) \neq Y)=\inf _{\text {fmeasurable }} P(f(X) \neq Y)
$$

Complexity:

- Memory: story $X$ is $O(n d)$
- Training time: 0
- Prediction: $O(n d)$ for each test point


## Linear models for classification



- Training set $\mathcal{S}=\left\{\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right)\right\} \subset \mathbb{R}^{d} \times\{-1,1\}$
- Fit a linear function

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

- The prediction on a new point $x \in \mathbb{R}^{d}$ is:

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

## Large-margin classifiers



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

$$
y f(x)
$$

- Large-margin classifiers fit a classifier by maximizing the margins on the training set:

$$
\min _{\beta} \sum_{i=1}^{n} \ell\left(y_{i} f_{\beta}\left(x_{i}\right)\right)+\lambda \beta^{\top} \beta
$$

for a convex, non-increasing loss function $\ell: \mathbb{R} \rightarrow \mathbb{R}+$

## Loss function examples



| Loss | Method | $\ell(u)$ |
| :---: | :---: | :---: |
| $0-1$ | none | $1(u \leq 0)$ |
| Hinge | Support vector machine (SVM) | $\max (1-u, 0)$ |
| Logistic | Logistic regression | $\log \left(1+e^{-u}\right)$ |
| Square | Ridge regression | $(1-u)^{2}$ |

## Ridge logistic regression [Le Cessie and van Houwelingen, 1992]

$$
\min _{\beta \in \mathbb{R}^{p}} J(\beta)=\sum_{i=1}^{n} \ln \left(1+e^{-y_{i} \beta^{\top} x_{i}}\right)+\lambda \beta^{\top} \beta
$$

- Can be interpreted as a regularized conditional maximum likelihood estimator
- No explicit solution, but smooth convex optimization problem that can be solved numerically by Newton-Raphson iterations:

$$
\beta^{\text {new }} \leftarrow \beta^{\text {old }}-\left[\nabla_{\beta}^{2} J\left(\beta^{\text {old }}\right)\right]^{-1} \nabla_{\beta} J\left(\beta^{\text {old }}\right)
$$

- Each iteration amounts to solving a weighted ridge regression problem, hence the name iteratively reweighted least squares (IRLS).
- Complexity $O$ (iterations * $\left(n d^{2}+d^{3}\right)$ )


## SVM [Boser et al., 1992]

$$
\min _{\beta \in \mathbb{R}^{p}} \sum_{i=1}^{n} \max \left(0,1-y_{i} \beta^{\top} x_{i}\right)+\lambda \beta^{\top} \beta
$$

- A non-smooth convex optimization problem (convex quadratic program)
- Equivalent to the dual problem

$$
\max _{\alpha \in \mathbb{R}^{n}} 2 \alpha^{\top} Y-\alpha^{\top} X X^{\top} \alpha \quad \text { s.t. } \quad 0 \leq \mathbf{y}_{i} \alpha_{i} \leq \frac{1}{2 \lambda} \text { for } i=1, \ldots, n
$$

- The solution $\beta^{*}$ of the primal is obtained from the solution $\alpha^{*}$ of the dual:

$$
\beta^{*}=X^{\top} \alpha^{*} \quad f_{\beta^{*}}(x)=\left(\beta^{*}\right)^{\top} x=\left(\alpha^{*}\right)^{\top} X x
$$

- Training complexity: $O\left(n^{2}\right)$ to store $X X^{\top}, O\left(n^{3}\right)$ to find $\alpha^{*}$
- Prediction: $O(d)$ for $\left(\beta^{*}\right)^{\top} x, O(n d)$ for $\left(\alpha^{*}\right)^{\top} X x$


## Outline

## (1) Introduction

(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: k-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning

4 Conclusion



## Model

- Learn a function $f: \mathbb{R}^{d} \rightarrow \mathbb{R}$ of the form

$$
f(x)=\sum_{i=1}^{n} \alpha_{i} K\left(x_{i}, x\right)
$$

- For a positive definite (p.d.) kernel $K: \mathbb{R}^{d} \times \mathbb{R}^{d} \rightarrow \mathbb{R}$, such as Linear $K\left(x, x^{\prime}\right)=x^{\top} x^{\prime}$
Polynomial $K\left(x, x^{\prime}\right)=\left(x^{\top} x^{\prime}+c\right)^{p}$
Gaussian $K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)$
$\operatorname{Min} / \max \quad K\left(x, x^{\prime}\right)=\sum_{i=1}^{d} \frac{\min \left(\left|x_{i}\right|,\left|x_{i}^{\prime}\right|\right)}{\max \left(\left|x_{i}\right|,\left|x_{i}^{\prime}\right|\right)}$


## Feature space

- A function $K: \mathbb{R}^{d} \times \mathbb{R}^{d} \rightarrow \mathbb{R}$ is a p.d. kernel if and only if there existe a mapping $\Phi: \mathbb{R}^{d} \rightarrow \mathbb{R}^{D}$, for some $D \in \mathbb{N} \cup\{+\infty\}$, such that

$$
\forall x, x^{\prime} \in \mathbb{R}^{d}, \quad K\left(x, x^{\prime}\right)=\Phi(x)^{\top} \Phi\left(x^{\prime}\right)
$$

- $f$ is then a linear function in $\mathbb{R}^{D}$ :

$$
f(x)=\sum_{i=1}^{n} \alpha_{i} K\left(x_{i}, x\right)=\sum_{i=1}^{n} \alpha_{i} \Phi\left(x_{i}\right)^{\top} \Phi(x)=\beta^{\top} \Phi(x)
$$

for $\beta=\sum_{i=1}^{n} \alpha_{i} \Phi\left(x_{i}\right)$.



## Learning



- We can learn $f(x)=\sum_{i=1}^{n} \alpha_{i} K\left(x_{i}, x\right)$ by fitting a linear model $\beta^{\top} \Phi(x)$ in the feature space
- Example: ridge regression / logistic regression / SVM

$$
\min _{\beta \in \mathbb{R}^{D}} \sum_{i=1}^{n} \ell\left(y_{i}, \beta^{\top} \Phi\left(x_{i}\right)\right)+\lambda \beta^{\top} \beta
$$

- But $D$ can be very large, even infinite...


## Kernel tricks

- $K\left(x, x^{\prime}\right)=\Phi(x)^{\top} \Phi\left(x^{\prime}\right)$ can be quick to compute even if $D$ is large (even infinite)
- For a set of training samples $\left\{x_{1}, \ldots, \mathbf{x}_{n}\right\} \subset \mathbb{R}^{d}$ let $K_{n}$ the $n \times n$ Gram matrix:

$$
\left[K_{n}\right]_{i j}=K\left(x_{i}, x_{j}\right)
$$

- For $\beta=\sum_{i=1}^{n} \alpha_{i} \Phi\left(x_{i}\right)$ we have

$$
\beta^{\top} \Phi\left(x_{i}\right)=[K \alpha]_{i} \quad \text { and } \quad \beta^{\top} \beta=\alpha^{\top} K \alpha
$$

- We can therefore solve the equivalent problem in $\alpha \in \mathbb{R}^{n}$

$$
\min _{\alpha \in \mathbb{R}^{n}} \sum_{i=1}^{n} \ell\left(y_{i},[K \alpha]_{i}\right)+\lambda \alpha^{\top} K \alpha
$$

## Example: kernel ridge regression (KRR)

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta
$$

- Solve in $\mathbb{R}^{D}$ :

$$
\hat{\beta}=\underbrace{\left(\Phi(X)^{\top} \Phi(X)+\lambda I\right)^{-1}}_{D \times D} \Phi(X)^{\top} Y
$$

- Solve in $\mathbb{R}^{n}$ :

$$
\hat{\alpha}=\underbrace{(K+\lambda I)^{-1}}_{n \times n} Y
$$

## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$



## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

$\operatorname{lambda}=1000$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=100$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

$\operatorname{lambda}=\mathbf{1 0}$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=1$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.1$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.01$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.001$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.0001$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $\mathbf{= 0 . 0 0 0 0 1}$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.000001$


## KRR with Gaussian RBF kernel

$$
\min _{\beta \in \mathbb{R}^{d}} \sum_{i=1}^{n}\left(y_{i}-\beta^{\top} \Phi\left(x_{i}\right)\right)^{2}+\lambda \beta^{\top} \beta \quad K\left(x, x^{\prime}\right)=\exp \left(\frac{\left\|x-x^{\prime}\right\|^{2}}{2 \sigma^{2}}\right)
$$

lambda $=0.0000001$


## Complexity

lambda $=1$


- Compute K: $O\left(d n^{2}\right)$
- Store $K: O\left(n^{2}\right)$
- Solve $\alpha$ : $O\left(n^{2 \sim 3}\right)$
- Compute $f(x)$ for one $x$ : $O(n d)$
- Unpractical for $n>10 \sim 100 k$


## Outline

(1) Introduction
(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning
- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## What is "large-scale"?

- Data cannot fit in RAM
- Algorithm cannot run on a single machine in reasonable time (algorithm-dependent)
- Sometimes even $O(n)$ is too large! (e.g., nearest neighbor in a database of $O(B+)$ items)
- Many tasks / parameters (e.g., image categorization in $O(10 M)$ classes)
- Streams of data



## Things to worry about

- Training time (usually offline)
- Memory requirements
- Test time
- Complexities so far

| Method | Memory | Training time | Test time |
| :---: | :---: | :---: | :---: |
| PCA | $O\left(d^{2}\right)$ | $O\left(n d^{2}\right)$ | $O(d)$ |
| $k$-means | $O(n d)$ | $O(n d k)$ | $O(k d)$ |
| Ridge regression | $O\left(d^{2}\right)$ | $O\left(n d^{2}\right)$ | $O(d)$ |
| kNN | $O(n d)$ | 0 | $O(n d)$ |
| Logistic regression | $O(n d)$ | $O\left(n d^{2}\right)$ | $O(d)$ |
| SVM, kernel methods | $O\left(n^{2}\right)$ | $O\left(n^{3}\right)$ | $O(n d)$ |

## Techniques for large-scale machine learning

- Good baselines:
- Subsample data and run standard method
- Split and run on several machines (depends on algorithm)
- Need to revisit standard algorithms and implementation, taking into account scalability

$n$
- Trade exactness for scalability
- Compress, sketch, hash data in a smart way


## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## Motivation

- Classical learning theory analyzes the trade-off between:
- approximation error (how well we approximate the true function)
- estimation errors (how well we estimate the parameters)

- But reaching the best trade-off for a given $n$ may be impossible with limited computational resources
- We should include in the trade-off the computational budget, and see which optimization algorithm gives the best trade-off!
- Seminal paper of Bottou and Bousquet [2008]


## Classical ERM setting

- Goal: learn a function $f: \mathbb{R}^{d} \rightarrow \mathcal{Y}(\mathcal{Y}=\mathbb{R}$ or $\{-1,1\})$
- $P$ unknown distribution over $\mathbb{R}^{d} \times \mathcal{Y}$
- Training set: $\mathcal{S}=\left\{\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right)\right\} \subset \mathbb{R}^{d} \times \mathcal{Y}$ i.i.d. following P
- Fix a class of functions $\mathcal{F} \subset\left\{f: \mathbb{R}^{d} \rightarrow \mathbb{R}\right\}$
- Choose a loss $\ell(y, f(x))$
- Learning by empirical risk minimization

$$
f_{n} \in \arg \min _{f \in \mathcal{F}} R_{n}[f]=\frac{1}{n} \sum_{i=1}^{n} \ell\left(Y_{i}, f\left(X_{i}\right)\right)
$$

- Hope that $f_{n}$ has a small risk:

$$
R\left[f_{n}\right]=E \ell\left(Y, f_{n}(X)\right)
$$

## Classical ERM setting

- The best possible risk is

$$
R^{*}=\min _{f: \mathbb{R}^{d} \rightarrow \mathcal{Y}} R[f]
$$

- The best achievable risk over $\mathcal{F}$ is

$$
R_{\mathcal{F}}^{*}=\min _{f \in \mathcal{F}} R[f]
$$

- We then have the decomposition

$$
R\left[f_{n}\right]-R^{*}=\underbrace{R\left[f_{n}\right]-R_{\mathcal{F}}^{*}}_{\text {estimation error } \epsilon_{\text {est }}}+\underbrace{R_{\mathcal{F}}^{*}-R_{*}}_{\text {approximation errror } \epsilon_{\text {app }}}
$$



## Optimization error

- Solving the ERM problem may be hard (when $n$ and $d$ are large)
- Instead we usually find an approximate solution $\tilde{f}_{n}$ that satisfies

$$
R_{n}\left[\tilde{f}_{n}\right] \leq R_{n}\left[f_{n}\right]+\rho
$$

- The excess risk of $\tilde{f}_{n}$ is then

$$
\epsilon=R\left[\tilde{f}_{n}\right]-R^{*}=\underbrace{R\left[\tilde{f}_{n}\right]-R\left[f_{n}\right]}_{\text {optimization error } \epsilon_{\text {opt }}}+\epsilon_{\text {est }}+\epsilon_{\text {app }}
$$

## A new trade-off

$$
\epsilon=\epsilon_{a p p}+\epsilon_{e s t}+\epsilon_{o p t}
$$

Problem

- Choose $\mathcal{F}, n, \rho$ to make $\epsilon$ as small as possible
- Subject to a limit on $n$ and on the computation time $T$

Table 1: Typical variations when $\mathcal{F}$, $n$, and $\rho$ increase.

|  |  | $\mathcal{F}$ | $n$ | $\rho$ |
| :--- | :--- | :---: | :---: | :---: |
| $\mathcal{E}_{\text {app }}$ | (approximation error) | $\searrow$ |  |  |
| $\mathcal{E}_{\text {est }}$ | (estimation error) | $\nearrow$ | $\searrow$ |  |
| $\mathcal{E}_{\text {opt }}$ | (optimization error) | $\cdots$ | $\cdots$ | $\nearrow$ |
| $T$ | (computation time) | $\nearrow$ | $\nearrow$ | $\searrow$ |

Large-scale or small-scale?

- Small-scale when constraint on $n$ is active
- Large-scale when constraint on $T$ is active


## Comparing optimization methods

$$
\min _{\beta \in \mathcal{B} \subset \mathbb{R}^{d}} R_{n}\left[f_{\beta}\right]=\sum_{i=1}^{n} \ell\left(y_{i}, f_{\beta}\left(x_{i}\right)\right)
$$

- Gradient descent (GD):

$$
\beta_{t+1} \leftarrow \beta_{t}-\eta \frac{\partial R_{n}\left(f_{\beta_{t}}\right)}{\partial \beta}
$$

- Second-order gradient descent (2GD), assuming Hessian $H$ known

$$
\beta_{t+1} \leftarrow \beta_{t}-H^{-1} \frac{\partial R_{n}\left(f_{\beta_{t}}\right)}{\partial \beta}
$$

- Stochastic gradient descent (SGD):

$$
\beta_{t+1} \leftarrow \beta_{t}-\frac{\eta}{t} \frac{\partial \ell\left(y_{t}, f_{\beta_{t}}\left(x_{t}\right)\right)}{\partial \beta}
$$

## Results [Bottou and Bousquet, 2008]

| Algorithm | Cost of one <br> iteration | Iterations <br> to reach $\rho$ | Time to reach <br> accuracy $\boldsymbol{\rho}$ | Time to reach <br> $\mathcal{E} \leq \boldsymbol{c}\left(\mathcal{E}_{\text {app }}+\boldsymbol{*}\right.$ |
| :--- | :---: | :---: | :---: | :---: |
| GD | $\mathcal{O}(n d)$ | $\mathcal{O}\left(\kappa \log \frac{1}{\rho}\right)$ | $\mathcal{O}\left(n d \kappa \log \frac{1}{\rho}\right)$ | $\mathcal{O}\left(\frac{d^{2} \kappa}{\varepsilon^{\kappa} / \alpha} \log ^{2} \frac{1}{\varepsilon}\right)$ |
| 2 GD | $\mathcal{O}\left(d^{2}+n d\right)$ | $\mathcal{O}\left(\log \log \frac{1}{\rho}\right)$ | $\mathcal{O}\left(\left(d^{2}+n d\right) \log \log \frac{1}{\rho}\right)$ | $\mathcal{O}\left(\frac{d^{2}}{\varepsilon^{2} / \alpha} \log \frac{1}{\varepsilon} \log \log \frac{1}{\varepsilon}\right)$ |
| SGD | $\mathcal{O}(d)$ | $\frac{\nu \kappa^{2}}{\rho}+\mathrm{o}\left(\frac{1}{\rho}\right)$ | $\mathcal{O}\left(\frac{d \nu \kappa^{2}}{\rho}\right)$ | $\mathcal{O}\left(\frac{d \nu \kappa^{2}}{\varepsilon}\right)$ |

- $\alpha \in[1 / 2,1]$ comes from the bound on $\varepsilon_{\text {est }}$ and depends on the data
- In the last column, $n$ and $\rho$ are optimized to reach $\epsilon$ for each method
- 2GD optimizes much faster than GD, but limited gain on the final performance limited by $\epsilon^{-1 / \alpha}$ coming from the estimation error
- SGD:
- Optimization speed is catastrophic
- Learning speed is the best, and independent of $\alpha$
- This suggests that SGD is very competitive (and has become the de facto standard in large-scale ML)


## Illustration

- Results: Linear SVM

$$
\ell(\hat{y}, y)=\max \{0,1-y \hat{y}\} \quad \lambda=0.0001
$$

|  | Training Time | Primal cost | Test Error |
| :--- | ---: | ---: | ---: |
| SVMLight | 23,642 secs | 0.2275 | $6.02 \%$ |
| SVMPerf | 66 secs | 0.2278 | $6.03 \%$ |
| SGD | 1.4 secs | 0.2275 | $6.02 \%$ |

- Results: Log-Loss Classifier

$$
\ell(\hat{y}, y)=\log (1+\exp (-y \hat{y})) \quad \lambda=0.00001
$$

Training Time Primal cost Test Error

| TRON(LibLinear, $\varepsilon=0.01)$ | 30 secs | 0.18907 | $5.68 \%$ |
| :--- | ---: | :--- | :--- |
| TRON(LibLinear, $\varepsilon=0.001)$ | 44 secs | 0.18890 | $5.70 \%$ |
| SGD | 2.3 secs | 0.18893 | $5.66 \%$ |

https://bigdata2013.sciencesconf.org/conference/bigdata2013/pages/bottou.pdf

## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## Motivation

- Affects scalability of algorithms, e.g., $O(n d)$ for kNN or $O\left(d^{3}\right)$ for ridge regression
- Hard to visualize
- (Sometimes) counterintuitive phenomena in high dimension, e.g., concentration of measure for Gaussian data



- Statistical inference degrades when $d$ increases (curse of dimension)


## Dimension reduction with PCA



- Projects data onto $k<d$ dimensions that captures the largest amount of variance
- Also minimizes total reconstruction errors:

$$
\min _{S_{k}} \sum_{i=1}^{n}\left\|x_{i}-\Pi_{S_{k}}\left(x_{i}\right)\right\|^{2}
$$

- But computational expensive: $O\left(n d^{2}\right)$
- No theoretical garantee on distance preservation


## Linear dimension reduction



$$
\underbrace{X^{\prime}}_{n \times k}=\underbrace{X}_{n \times d} \times \underbrace{R}_{d \times k}
$$

- Can we find $R$ efficiently?
- Can we preserve distances?

$$
\forall i, j=1, \ldots, n, \quad\left\|f\left(x_{i}\right)-f\left(x_{j}\right)\right\| \approx\left\|x_{i}-x_{j}\right\|
$$

- Note: when $d>n$, we can take $k=n$ and preserve all distances exactly (kernel trick)


## Random projections

Simply take a random projection matrix:

$$
f(x)=\frac{1}{\sqrt{k}} R^{\top} x \quad \text { with } \quad R_{i j} \sim \mathcal{N}(0,1)
$$

## Theorem [Johnson and Lindenstrauss, 1984]

For any $\epsilon>0$ and $n \in \mathbb{N}$, take

$$
k \geq 4\left(\epsilon^{2} / 2-\epsilon^{3} / 3\right)^{-1} \log (n) \approx \epsilon^{-2} \log (n)
$$

Then the following holds with probabiliy at least $1-1 / n$ :
$\forall i, j=1, \ldots, n \quad(1-\epsilon)\left\|x_{i}-x_{j}\right\|^{2} \leq\left\|f\left(x_{i}\right)-f\left(x_{j}\right)\right\|^{2} \leq(1+\epsilon)\left\|x_{i}-x_{j}\right\|^{2}$

- $k$ does not depend on $d$ !
- $n=1 M, \epsilon=0.1 \Longrightarrow k \approx 5 K$
- $n=1 B, \epsilon=0.1 \Longrightarrow k \approx 8 K$


## Proof $(1 / 3)$

- For a single dimension, $q_{j}=r_{j}^{\top} u$ :

$$
\begin{aligned}
E\left(q_{j}\right) & =E\left(r_{j}\right)^{\top} u=0 \\
E\left(q_{j}\right)^{2} & =u^{\top} E\left(r_{j} r_{j}^{\top}\right) u=\|u\|^{2}
\end{aligned}
$$

- For the $k$-dimensional projection $f(u)=1 / \sqrt{k} R^{\top} u$ :

$$
\begin{aligned}
\|f(u)\|^{2} & =\frac{1}{k} \sum_{j=1}^{k} q_{j}^{2} \sim \frac{\|u\|^{2}}{k} \chi^{2}(k) \\
E\|f(u)\|^{2} & =\frac{1}{k} \sum_{j=1}^{k} E\left(q_{j}^{2}\right)=\|u\|^{2}
\end{aligned}
$$

- Need to show that $\|f(u)\|^{2}$ is concentrated around its mean


## Proof $(2 / 3)$

$$
\begin{aligned}
P & {\left[\|f\|^{2}>(1+\epsilon)\|u\|^{2}\right] } \\
& =P\left[\chi^{2}(k)>(1+\epsilon) k\right] \\
& =P\left[e^{\lambda \chi^{2}(k)}>e^{\lambda(1+\epsilon) k}\right] \\
& \leq E\left[e^{\lambda \chi^{2}(k)}\right] e^{-\lambda(1+\epsilon) k} \\
& =(1-2 \lambda)^{-\frac{k}{2}} e^{-\lambda(1+\epsilon) k} \\
& =\left((1+\epsilon) e^{-\epsilon}\right)^{k / 2} \\
& \leq e^{-\left(\epsilon^{2} / 2-\epsilon^{3} / 3\right) k / 2} \\
& =n^{-2}
\end{aligned}
$$

(Markov)
(MGF of $\chi^{2}(k)$ for $0 \leq \lambda \leq 1 / 2$ )
(take $\lambda=\epsilon / 2(1+\epsilon)$ )
(use $\log (1+x) \leq x-x^{2} / 2+x^{3} / 3$ )
(take $k=4\left(\epsilon^{2} / 2-\epsilon^{3} / 3\right) \log (n)$ )

Similarly we get

$$
P\left[\|f\|^{2}<(1-\epsilon)\|u\|^{2}\right]<n^{-2}
$$

## Proof $(3 / 3)$

- Apply with $u=x_{i}-x_{j}$ and use linearity of $f$ to show that for an $\left(x_{i}, x_{j}\right)$ pair, the probability of large distortion is $\leq 2 n^{-2}$
- Union bound: for all $n(n-1) / 2$ pairs, the probability that at least one has large distortion is smaller than

$$
\frac{n(n-1)}{2} \times \frac{2}{n^{2}}=1-\frac{1}{n}
$$

## Scalability

- $n=O(1 B) ; d=O(1 M) \Longrightarrow k=O(10 K)$
- Memory: need to store $R, O(d k) \approx 40 G B$
- Computation: $X \times R$ in $O(n d k)$
- Other random matrices $R$ have similar properties but better scalability, e.g.:
- "add or subtract" [Achlioptas, 2003], 1 bit/entry, size $\approx 1,25 G B$

$$
R_{i j}= \begin{cases}+1 & \text { with probability } 1 / 2 \\ -1 & \text { with probability } 1 / 2\end{cases}
$$

- Fast Johnson-Lindenstrauss transform [Ailon and Chazelle, 2009] where $R=P H D$, compute $f(x)$ in $O(d \log d)$



## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## Motivation



## Fourier feature space

Example: Gaussian kernel

$$
\begin{aligned}
e^{-\frac{\left\|x-x^{\prime}\right\|^{2}}{2}} & =\frac{1}{(2 \pi)^{\frac{d}{2}}} \int_{\mathbb{R}^{d}} e^{i \omega^{\top}\left(x-x^{\prime}\right)} e^{-\frac{\|\omega\|^{2}}{2}} d \omega \\
& =E_{\omega} \cos \left(\omega^{\top}\left(x-x^{\prime}\right)\right) \\
& =E_{\omega, b}\left[2 \cos \left(\omega^{\top} x+b\right) \cos \left(\omega^{\top} x^{\prime}+b\right)\right]
\end{aligned}
$$

with

$$
\omega \sim p(d \omega)=\frac{1}{(2 \pi)^{\frac{d}{2}}} e^{-\frac{\|\omega\|^{2}}{2}} d \omega, \quad b \sim \mathcal{U}([0,2 \pi]) .
$$

This is of the form $K\left(x, x^{\prime}\right)=\Phi(x)^{\top} \Phi\left(x^{\prime}\right)$ with $D=+\infty$ :

$$
\Phi: \mathbb{R}^{d} \rightarrow L_{2}\left(\left(\mathbb{R}^{d}, p(d \omega)\right) \times([0,2 \pi], \mathcal{U})\right)
$$

## Random Fourier features [Rahimi and Recht, 2008]

- For $i=1, \ldots, k$, sample randomly:

$$
\left(\omega_{i}, b_{i}\right) \sim p(d \omega) \times \mathcal{U}([0,2 \pi])
$$

- Create random features:

$$
\forall x \in \mathbb{R}^{d}, \quad f_{i}(x)=\sqrt{\frac{2}{k}} \cos \left(\omega_{i}^{\top} x+b_{i}\right)
$$




## Random Fourier features [Rahimi and Recht, 2008]

For any $x, x^{\prime} \in \mathbb{R}^{d}$, it holds

$$
\begin{aligned}
E\left[f(x)^{\top} f\left(x^{\prime}\right)\right] & =\sum_{i=1}^{k} E\left[f_{i}(x) f_{i}\left(x^{\prime}\right)\right] \\
& =\frac{1}{k} \sum_{i=1}^{k} E\left[2 \cos \left(\omega^{\top} x+b\right) \cos \left(\omega^{\top} x^{\prime}+b\right)\right] \\
& =K\left(x, x^{\prime}\right)
\end{aligned}
$$

and by Hoeffding's inequality,

$$
P\left[\left|f(x)^{\top} f\left(x^{\prime}\right)-K\left(x, x^{\prime}\right)\right|>\epsilon\right] \leq 2 e^{-\frac{k \epsilon^{2}}{2}}
$$

This allows to approximate learning with the Gaussian kernel with a simple linear model in $k$ dimensions!

## Generalization

A translation-invariant (t.i.) kernel is of the form

$$
K\left(x, x^{\prime}\right)=\varphi\left(x-x^{\prime}\right)
$$

## Bochner's theorem

For a continuous function $\varphi: \mathbb{R}^{d} \rightarrow \mathbb{R}, K$ is p.d. if and only if $\varphi$ is the Fourier-Stieltjes transform of a symmetric and positive finite Borel measure $\mu \in M\left(\mathbb{R}^{d}\right)$ :

$$
\varphi(x)=\int_{\mathbb{R}^{d}} e^{-i \omega^{\top} x} d \mu(\omega)
$$

Just sample $\omega_{i} \sim \frac{d \mu(\omega)}{\mu\left(\mathbb{R}^{d}\right)}$ and $b_{i} \sim \mathcal{U}([0,2 \pi])$ to approximate any t.i. kernel $K$ with random features

$$
\sqrt{\frac{2}{k}} \cos \left(\omega_{i}^{\top} x+b_{i}\right)
$$

## Examples

$$
K\left(x, x^{\prime}\right)=\varphi\left(x-x^{\prime}\right)=\int_{\mathbb{R}^{d}} e^{-i \omega^{\top}\left(x-x^{\prime}\right)} d \mu(\omega)
$$

| Kernel | $\varphi(x)$ | $\mu(d \omega)$ |
| :---: | :---: | :---: |
| Gaussian | $\exp \left(-\frac{\\|x\\|^{2}}{2}\right)$ | $(2 \pi)^{-d / 2} \exp -\left(\frac{\\|\omega\\|^{2}}{2}\right)$ |
| Laplace | $\exp \left(-\\|x\\|_{1}\right)$ | $\prod_{i=1}^{k} \frac{1}{\pi\left(1+\omega_{i}^{2}\right)}$ |
| Cauchy | $\prod_{i=1}^{k} \frac{2}{1+\mathrm{x}_{i}^{2}}$ | $e^{-\\|\omega\\|_{1}}$ |

## Performance [Rahimi and Recht, 2008]

| Dataset | Fourier+LS | Binning+LS | CVM | Exact SVM |
| :--- | :--- | :--- | :--- | :--- |
| CPU | $3.6 \%$ | $5.3 \%$ | $5.5 \%$ | $11 \%$ |
| regression | 20 secs | 3 mins | 51 secs | 31 secs |
| 6500 instances 21 dims | $D=300$ | $P=350$ |  | ASVM |
| Census | $5 \%$ | $7.5 \%$ | $8.8 \%$ | $9 \%$ |
| regression | 36 secs | 19 mins | 7.5 mins | 13 mins |
| 18,000 instances 119 dims | $D=500$ | $P=30$ |  | SVMTorch |
| Adult | $14.9 \%$ | $15.3 \%$ | $14.8 \%$ | $15.1 \%$ |
| classification | 9 secs | 1.5 mins | 73 mins | 7 mins |
| 32,000 instances 123 dims | $D=500$ | $P=30$ |  | SVM $^{\text {light }}$ |
| Forest Cover | $11.6 \%$ | $2.2 \%$ | $2.3 \%$ | $2.2 \%$ |
| classification | 71 mins | 25 mins | 7.5 hrs | 44 hrs |
| 522,000 instances 54 dims | $D=5000$ | $P=50$ |  | libSVM |
| KDDCUP99 (see footnote) | $7.3 \%$ | $7.3 \%$ | $6.2 \%(18 \%)$ | $8.3 \%$ |
| classification | 1.5 min | 35 mins | $1.4 \operatorname{secs}(20$ secs $)$ | $<1 \mathrm{~s}$ |
| $4,900,000$ instances 127 dims | $D=50$ | $P=10$ |  | SVM+sampling |

## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching
(4) Conclusion


## Motivation



- Database $\mathcal{S}=\left\{x_{1}, \ldots, x_{n}\right\} \subset \mathbb{R}^{d}$, query $q \in \mathbb{R}^{d}$
- Naively: $O(n d)$ to compute distances $\left\|q-x_{i}\right\|$ and find the smallest one
- For $n=1 B, d=10 k$, it takes 15 hours
- Projections $\mathbb{R}^{d} \rightarrow \mathbb{R}^{k}$ with $k<d$ is not good enough if $n$ is large


## ANN

Given $\epsilon>0$, the approximate nearest neighbor (ANN) problem is:
Find $y \in \mathcal{S}$ such that $\|q-y\| \leq(1+\epsilon) \min _{x \in \mathcal{S}}\|q-x\|$
Two popular ANN approaches
(1) Tree approaches

- Recursively partition the data: Divide and Conquer
- Expected query time: $O(\log (n))$
- Many variants: KDtree, Balltree, PCA-tree, Vantage Point tree
- Shown to perform very well in relatively low-dim data
(2) Hashing approaches
- Each image in database represented as a code
- Significant reduction in storage
- Expected query time: $O(1)$ or $O(n)$
- Compact codes preferred


## KD tree



- Axis-parallel splits
- Along the direction of largest variance
- Split along the median $\Longrightarrow$ balanced partitioning
- Split recursively until each node has a single data point


## Search in a KD tree



- Finds the leaf of the query in $O(\log (n))$
- But backtracking is needed to visit other leaves surrounding the cell
- As $d$ increases, the number of leaves to visit grows exponentially
- Complexity: $O(n d \log (n))$ to build the tree, $O(n d)$ to store the original data
- Works fine up to $d=10 \sim 100$


## Variants



## Variants

Ball tree

PCA tree


right


## Binary code using multiple hashing



No recursive partitioning, unlike trees
ANN with codes:
(1) Choose a set of binary hashing functions to design a binary code
(2) Index the database $=$ compute codes for all points
(3) Querying: compute the code of the query, and retrieve the points with similar codes

## Hashing

A hash function is a function $h: \mathcal{X} \rightarrow \mathcal{Z}$ where

- $\mathcal{X}$ is the set of data ( $\mathbb{R}^{d}$ for us)
- $\mathcal{Z}=\{1, \ldots, N\}$ is a finite set of codes

https://en.wikipedia.org/wiki/Hash_function
There is a collision when $h(x)=h\left(x^{\prime}\right)$ for two different entries $x \neq x^{\prime}$


## Locality sensitive hashing (LSH)

- Let a random hash function $h: \mathcal{X} \rightarrow \mathcal{Z}$
- It is a LSH with respect to a similarity function $\operatorname{sim}\left(x, x^{\prime}\right)$ on $\mathcal{X}$ if there exists a monotonically increasing function $f: \mathbb{R} \rightarrow[0,1]$ such that:

$$
\forall x, x^{\prime} \in \mathcal{X}, \quad P\left[h(x)=h\left(x^{\prime}\right)\right]=f\left(\operatorname{sim}\left(x, x^{\prime}\right)\right)
$$

- "Probability of collision increases with similarity"



## Example: simHash

$$
\begin{gathered}
\boldsymbol{r}^{\boldsymbol{T} \boldsymbol{x}>\mathbf{0}} \vdots \\
r \in \mathbb{R}^{d} \sim \mathcal{N}(0, \text { ld }) \quad h_{r}(x)= \begin{cases}1 & \text { if } r^{\top} x \geq 0 \\
0 & \text { otherwise }\end{cases} \\
P\left[h_{r}(x)=h_{r}\left(x^{\prime}\right)\right]=1-\frac{\theta}{\pi}
\end{gathered}
$$

LSH with respect to the cosine similarity $\operatorname{sim}\left(x, x^{\prime}\right)=\cos (\theta)$ [Goemans and Williamson, 1995].

## ANN with LSH



- $h_{i}(q)=h_{i}(x)$ implies high similarity (locality sensitive)


## ANN with LSH

Table 1

| $h_{1}^{1}$ | $\cdots$ | $h_{K}^{1}$ | Buckets |
| :--- | :--- | :--- | :--- |
| 00 | $\cdots$ | 00 | $\cdots$ |
| 00 | $\cdots$ | 01 | $0 \ldots$ |
| 00 | $\cdots$ | 10 | Empty |
| $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
| 11 | $\cdots$ | 11 | $\cdots$ |

Table L

| $h_{1}^{L}$ | $\cdots$ | $h_{K}^{L}$ | Buckets |
| :--- | :--- | :--- | :--- |
| 00 | $\cdots$ | 00 | $-\cdots$ |
| 00 | $\cdots$ | 01 | $0 \ldots$ |
| 00 | $\cdots$ | $\mathbf{1 0}$ | 0 |
| $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
| 11 | $\cdots$ | 11 | Empty |

- $h_{i}(q)=h_{i}(x)$ implies high similarity (locality sensitive)
- Use $K$ contenations, repeated in $L$ tables
- Querying: report union of $K$ buckets
- Choice of $K$ and $L$ :
- Large $m$ increases precision but decreases recall
- Large $L$ increases recall but also storage
- Optimization is possible to minimize run-time for a given application


## LSH for $\left\|x-x^{\prime}\right\|_{s}$ ?

$$
h_{k}(x)=\left\lfloor\frac{w_{k}^{\top} x+b_{k}}{t}\right\rfloor \quad w_{k} \sim \prod_{i=1}^{d} P_{s}\left(w_{k}^{i}\right), \quad b_{k} \sim \mathcal{U}([0, t])
$$



- $P_{s}$ a $s$-stable distribution, i.e., for any $x \in \mathbb{R}^{d}$, and any $w$ i.i.d. with $w^{i} \sim P_{s}, x^{\top} w \sim\|x\|_{s} w^{1}$.
- $s$-stable distributions exist for $p \in(0,2]$ :
- Gaussian $\mathcal{N}(0,1)$ is 2 -stable
- Cauchy $d x /\left(\pi\left(1+x^{2}\right)\right)$ is 1-stable
- Then $P\left[h_{k}(x)=h_{k}\left(x^{\prime}\right)\right]$ increases as $\left\|x-x^{\prime}\right\|_{s}$ decreases


## Outline

## (1) Introduction

(2) Standard machine learning
(3) Large-scale machine learning

- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## Motivation

- The hashing / LSH trick is a fast random projection to compact binary codes
- Initially proposed for ANN problems, it can also be used for more general learning problems
- It is particularly effective when data are first converted to huge binary vectors, using a specific similarity measure (the resemblance).
- Applications: texts, time series, images...


## Shingling and resemblance

- Given some input space $\mathcal{X}$ (e.g., texts, times series...), a shingling is a representation as large binary vector

$$
x \in\{0,1\}^{D}
$$

- Equivalently, represent $x$ as a subset of $S_{x} \subset \Omega=\{0, \ldots, D-1\}$
- Example: represent a text by the set of $w$-shingles it contains, i.e., sequences of $w$ words. Typically, $w=5,10^{5}$ words, $D=10^{2} 5$, but very sparse.
- A common measure of similarity between two such vectors is the resemblance (a.k.a. Jaccart or Tanimoto similarity):

$$
R\left(x_{1}, x_{2}\right)=\frac{\left|S_{1} \cap S_{2}\right|}{\left|S_{1} \cup S_{2}\right|}
$$

- But computing $R\left(x_{1}, x_{2}\right)$ is expensive, and not scalable for NN search or machine learning


## Minwise hashing

- Let $\pi \in \mathbb{S}_{D}$ be a random permutation of $\Omega$
- Let $h_{\pi}:\{0,1\}^{D} \rightarrow \Omega$ assign to $S \subset \Omega$ the smallest index of $\pi(S)$ :

$$
h_{\pi}(x)=\min \left\{\pi(i): i \in S_{x}\right\}
$$

## Theorem [Broder, 1997]

Minwise hashing is a LSH with respect to the resemblance:

$$
P\left[h_{\pi}\left(x_{1}\right)=h_{\pi}\left(x_{2}\right)\right]=R\left(x_{1}, x_{2}\right)
$$

Proof:

- The smallest index $\min \left(h_{\pi}\left(x_{1}\right), h_{\pi}\left(x_{2}\right)\right)$ correspond a random element of $S_{1} \cup S_{2}$
- $h_{\pi}\left(x_{1}\right)=h_{\pi}\left(x_{2}\right)$ if it is in $S_{1} \cap S_{2}$
- This happens with probability $R\left(x_{1}, x_{2}\right)$


## Applications of minwise hashing

- If we pick $k$ random permutations, we can represent $x$ by $\left(h_{1}(x), \ldots, h_{k}(x)\right) \in\{0,1\}^{D k}$
- Used for ANN, using the general LSH technique discussed earlier
- Learning linear models as an approximation to learning a nonlinear function with the resemblance kernel ${ }^{1}$
- Various tricks to improve scalability
- b-bit minwise hashing [Li and König, 2010]: only keep the last $b$ bits of $h_{\pi}(x)$, which reduces the dimensionality of the hashed matrix to $2^{b} k$
- One-permutation hashing [Li et al., 2012]: use a single permutation, keep the smallest index in each consecutive block of size $k$


[^0]
## Hash kernel [Shi et al., 2009]

- Goal: improve the scalability of random projections or minwise hashing, both in memory (sparsity) and processing time
- Simple idea:
- Let $h:[1, d] \rightarrow[1, k]$ a hash function
- For $x \in \mathbb{R}^{d}$ (or $\{0,1\}^{d}$ ) let $\Phi(x) \in \mathbb{R}^{k}$ with

$$
\forall i=1, \ldots, k \quad \Phi_{i}(x)=\sum_{j \in[1, d]: h(j)=i} x_{j}
$$

- "Accumulate coordinates $i$ of $x$ for which $h(i)$ is the same
- Repeat $L$ times and concatenate if needed, to limit the effect of collisions
- Advantages
- No memory needed for projections (vs. LSH)
- No need for dictionnary (just a hash function that can hash anything)
- Sparsity preserving


## Outline

(1) Introduction
(2) Standard machine learning

- Dimension reduction: PCA
- Clustering: $k$-means
- Regression: ridge regression
- Classification: kNN, logistic regression and SVM
- Nonlinear models: kernel methods
(3) Large-scale machine learning
- Scalability issues
- The tradeoffs of large-scale learning
- Random projections
- Random features
- Approximate NN
- Shingling, hashing, sketching

4 Conclusion

## What we saw

- Most standard ML algorithms do not scale to modern, large-scale problems
- They are being revisited with scalability as new constraint, both in theory and in practice
- Generally, trading accuracy for fast approximations can be beneficial:
- Optimization by SGD
- Random projections, sketching
- Need to understand mathematics, statistics, algorithms, hardware


## What we did not see

A lot!

- Hardware (distributed computing and storage, GPU, ...)
- Data streams
- Other models like deep learning or graphical models
- Other learning paradigms like reinforcement learning
- A lot of recent results (this is a very active research field!)


## MERCI!

## References I

D. Achlioptas. Database-friendly random projections: Johnson-lindenstrauss with binary coins. J. Comput. Syst. Sci., 66(4):671-687, 2003. doi: 10.1016/S0022-0000(03)00025-4. URL http://dx.doi.org/10.1016/S0022-0000(03)00025-4.
N. Ailon and B. Chazelle. The fast Johnson-Lindenstrauss transform and approximate nearest neighbors. SIAM J. Comput., 39(1):302-322, 2009. doi: 10.1137/060673096. URL http://dx.doi.org/10.1137/060673096.
B. E. Boser, I. M. Guyon, and V. N. Vapnik. A training algorithm for optimal margin classifiers. In Proceedings of the 5th annual ACM workshop on Computational Learning Theory, pages 144-152, New York, NY, USA, 1992. ACM Press. URL http://www.clopinet.com/isabelle/Papers/colt92.ps.Z.
L. Bottou and O. Bousquet. The tradeoffs of large scale learning. In J. C. Platt, D. Koller, Y. Singer, and S. T. Roweis, editors, Adv. Neural. Inform. Process Syst., volume 20, pages 161-168. Curran Associates, Inc., 2008. URL http://papers.nips.cc/paper/3323-the-tradeoffs-of-large-scale-learning.pdf.
A. Z. Broder. On the resemblance and containment of documents. In Proceedings of the Compression and Complexity of Sequences, pages 21-29, 1997. doi: 10.1109/SEQUEN.1997.666900. URL http://dx.doi.org/10.1109/SEQUEN. 1997.666900.
M. X. Goemans and D. P. Williamson. A general approximation technique for constrained forest problems. SIAM J. Comput., 24(2):296-317, apr 1995. doi: 10.1137/S0097539793242618. URL http://dx.doi.org/10.1137/S0097539793242618.

## References II

W. B. Johnson and J. Lindenstrauss. Extensions of lipschitz mappings into a hilbert space. Contemp. Math., 26:189-206, 1984. doi: 10.1090/conm/026/737400. URL http://dx.doi.org/10.1090/conm/026/737400.
S. Le Cessie and J. C. van Houwelingen. Ridge estimators in logistic regression. Appl. Statist., 41(1):191-201, 1992. URL http://www.jstor.org/stable/2347628.
P. Li and A. C. König. b-bit minwise hashing. In WWW, pages 671-680, Raleigh, NC, 2010.
P. Li, A. O., and C. hui Z. One permutation hashing. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 25, pages 3113-3121. Curran Associates, Inc., 2012. URL http://papers.nips.cc/paper/4778-one-permutation-hashing.pdf.
A. Rahimi and B. Recht. Random features for large-scale kernel machines. In J. Platt, D. Koller, Y. Singer, and S. Roweis, editors, Adv. Neural. Inform. Process Syst., volume 20, pages 1177-1184. Curran Associates, Inc., 2008. URL http://papers.nips.cc/paper/ 3182-random-features-for-large-scale-kernel-machines.pdf.
Q. Shi, J. Petterson, G. Dror, J. Langford, A. Smola, and S. Vishwanathan. Hash kernels for structured data. Journal of Machine Learning Research, 10:2615-2637, 2009.
C. Stone. Consistent nonparametric regression. Ann. Stat., 8:1348-1360, 1977. URL http://links.jstor.org/sici?sici=0090-5364\(197707\)5\%3A4\<595\%3ACNR\>2. $0 . C 0 \% 3 B 2-0$.


[^0]:    ${ }^{1}$ This shows in particular that the resemblance is positive definite

