Statistical Machine Learning for Data Science

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DATA 558

Week 7

Supervised learning

General objective

Let $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \{1, \ldots, k\}$ be labelled training examples

$$\min_{B \in \mathbb{R}^{d \times k}} \quad \lambda \, \Omega(B) + \frac{1}{n} \sum_{i=1}^{n} L\big(y_i, B^T x_i\big)$$

Large-scale setting

$$n \gg 1, \quad d \gg 1, \quad k \gg 1$$

Gradient descent

Gradient descent

Grouping the regularization penalty and the empirical risk in the objective

$$\nabla_B F(B) = \frac{1}{n} \sum_{i=1}^{n} \left\{ n\lambda \, \Omega(B) + L\left(y_i, B^T x_i\right) \right\}$$

Gradient descent

Gradient descent

Grouping the regularization penalty and the empirical risk, and expanding the sum onto the examples

$$\nabla_B F(B) = \frac{1}{n} \sum_{i=1}^{n} \left\{ n\lambda \, \Omega(B) + L\left(y_i, B^T x_i\right) \right\}$$

$$= \nabla_B \left\{ \frac{1}{n} \sum_{i=1}^{n} L(B; x_i, y_i) \right\}$$

Gradient descent

Gradient descent

- **Initialize**: $B = 0$
- **Iterate**:

$$
\begin{aligned}
B_{t+1} &= B_t - \eta_t \nabla F(B) \\
&= B_t - \eta_t \nabla_B \left\{ \frac{1}{n} \sum_{i=1}^{n} L(B; x_i, y_i) \right\}
\end{aligned}
$$

Gradient descent

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\end{aligned}
$$

Gradient descent

Strengths and weaknesses

- Strength: robust to setting of step-size sequence (line-search)
- Weakness: demanding disk/memory requirements

Tuning the step-size

Initial step-size estimate

- **standardize the data**
- use the formula

$$\eta_0 \propto \frac{1}{L}\,, \quad \text{where } L = \text{maximum-eigenvalue}\left(\frac{1}{n}X^T X\right) + \lambda$$

Practical advice

- Subsample the dataset
- Python $\rightarrow$ `largest-eigh`

Gradient descent with adaptive step-size

- **Initialize**: $B_0 = 0$.
- **Iterate**:

  Find η_t with backtracking rule.

$$
\begin{aligned}
B_{t+1} &= B_t - \eta_t \nabla_B F(B) \\
&= B_t - \eta_t \nabla_B \left\{ \frac{1}{n} \sum_{i=1}^{n} L(B; x_i, y_i) \right\}
\end{aligned}
$$

Fast Gradient Method

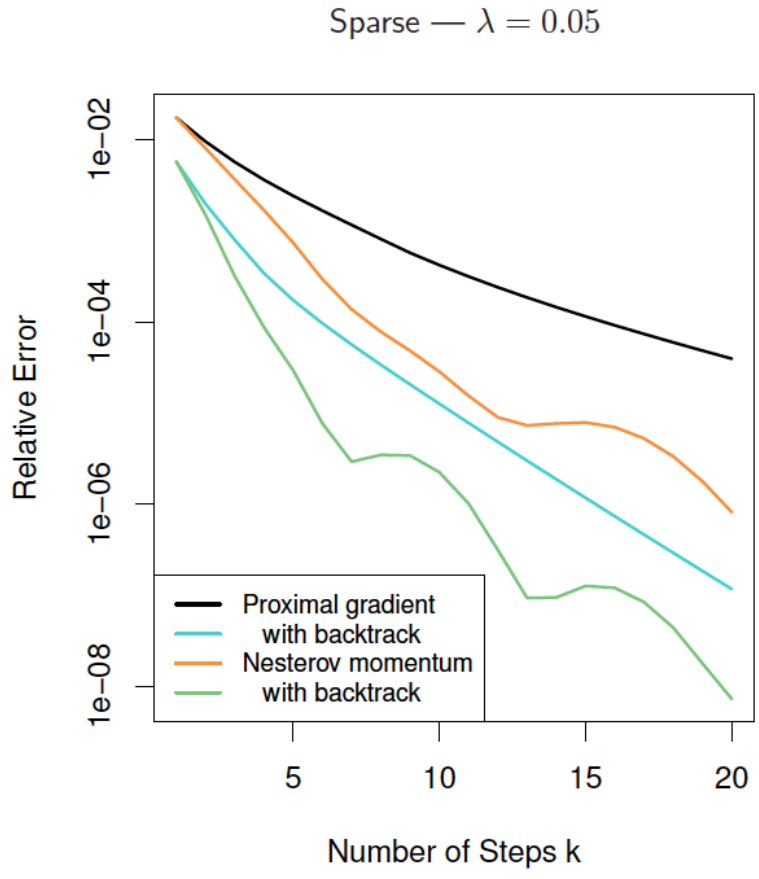
- **Initialize**: $B = 0$ and $\theta_0 = 0$.
- **Iterate**:

  Find η_t with backtracking rule.

$$B_{t+1} = \theta_t - \eta_t \nabla_\theta F(\theta)$$

$$\theta_{t+1} = B_{t+1} + \frac{t}{t+3}(B_{t+1} - B_t)$$

Accelerated Gradient Method



Performance of the gradient descent versus accelerated gradient on a regression problem.

Large-scale supervised learning

General form

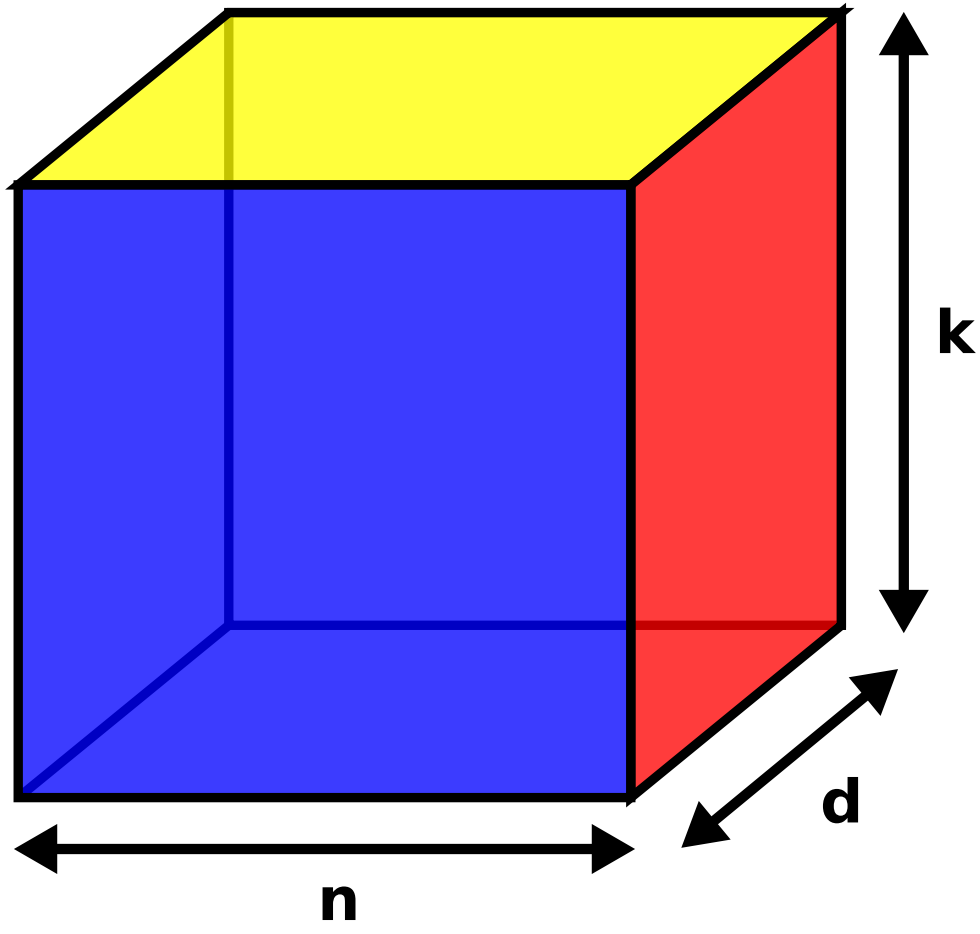
Let $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \{1, \ldots, k\}$ be labelled training examples

$$\min_{B \in \mathbb{R}^{d \times k}} \quad \lambda \, \Omega(B) + \frac{1}{n} \sum_{i=1}^{n} L\big(y_i, B^T x_i\big)$$

Problem: minimizing such objectives in the **large-scale** setting

$$n \gg 1, \quad d \gg 1, \quad k \gg 1$$

Machine learning cuboid



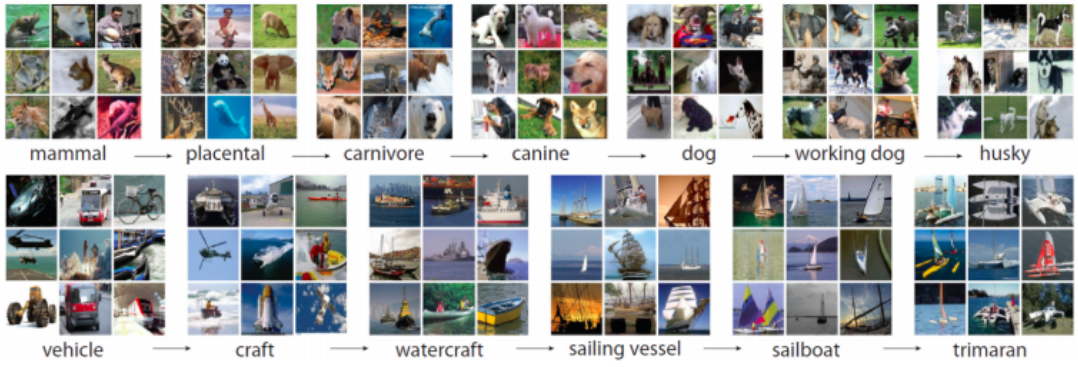
An example: ImageNet dataset

ImageNet dataset

- Large number of images/examples: $n = 17,000,000$
- Large number of pixels/image: $d = 200,030$
- Large number of categories: $k = 10,000$

Zoom on the ImageNet Dataset

Hierarchy of classes:



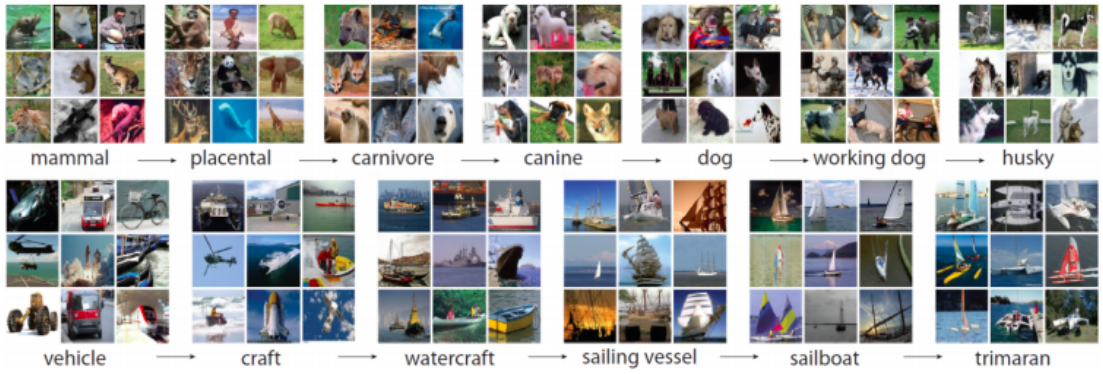
Deng, Dong, Socher, Li, Li and Fei-Fei, "Imagenet: a large-scale hierarchical image database", CVPR'09.

Fine-grained subsets: generally more practical problems

→ Fungus: 134 classes, 90K images

Zoom on the ImageNet Dataset

Hierarchy of classes:



Deng, Dong, Socher, Li, Li and Fei-Fei, "Imagenet: a large-scale hierarchical image database", CVPR'09.

Fine-grained subsets: generally more practical problems

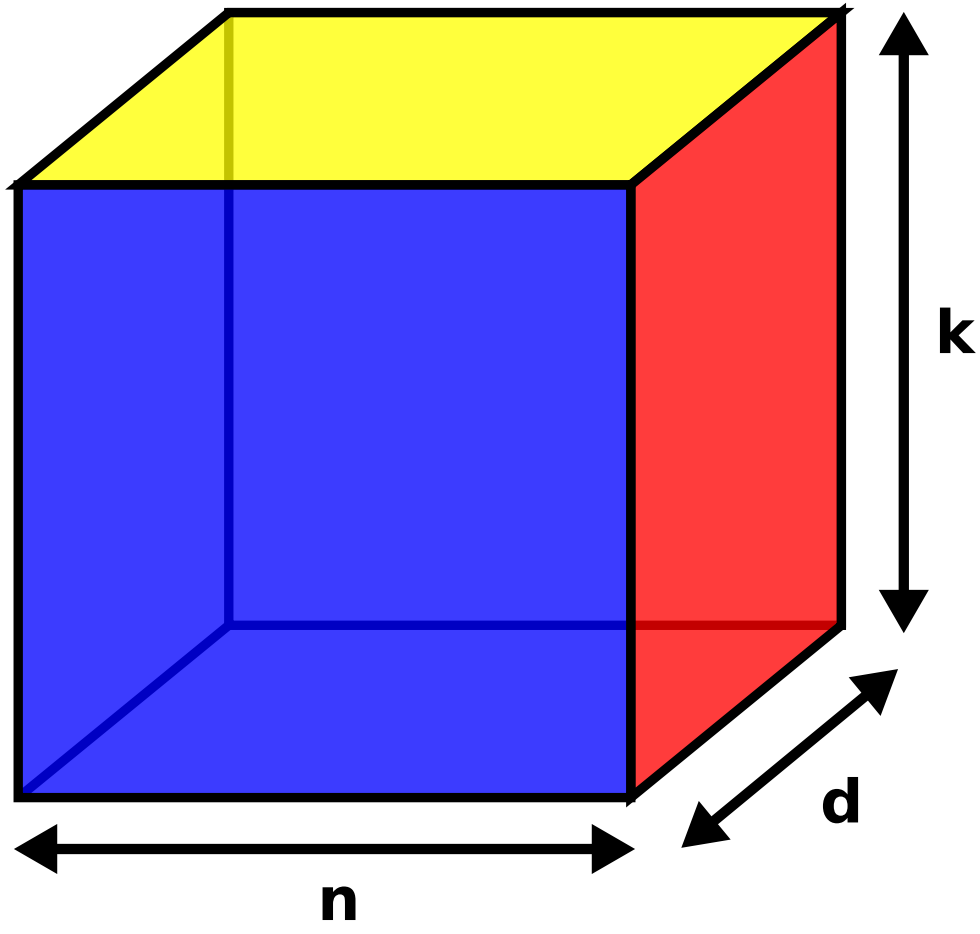
→ Vehicle: 262 classes, 226K images

Strategies for large-scale problems

Strategy: divide-and-conquer

Break the large learning problem into small and easy pieces

Machine learning cuboid



Aggregation or Decomposition principles

Aggregation or Decomposition principles

- Decomposition over examples: Stochastic gradient descent
- Decomposition over categories: One-versus-rest strategy
- Decomposition over features: Coordinate descent

Decomposition over examples

Stochastic gradient descent

- Bru, 1890: algorithm to adjust a slant θ of cannon in order to obtain a specified range r by trial and error, firing one shell after another

$$\theta_t = \theta_{t-1} - \frac{\eta_0}{t}(r - r_t)$$

- Perceptron, Rosenblatt, 1957

$$\begin{aligned} \beta_t &= \beta_{t-1} - \eta_t(y_t \phi(x_t)) && \text{if } y_t \phi(x_t) \leq 0 \\ &= \beta_{t-1} && \text{otherwise} \end{aligned}$$

Decomposition over examples

Stochastic gradient descent

- Bru, 1890: algorithm to adjust a slant θ of cannon in order to obtain a specified range r by trial and error
- Perceptron, Rosenblatt, 1957
- 60s-70s: extensions in learning, optimal control, and adaptive signal processing
- 80s-90s: extensions to non-convex learning problems
- see "Efficient backprop" in *Neural networks: Tricks of the trade*, LeCun et al., 1998, for wise advice and overview on sgd algorithms

Decomposition over examples

Stochastic gradient descent

- **Initialize**: $B = 0$
- **Iterate**: pick an example (x_t, y_t)

$$B_{t+1} = B_t - \eta_t \underbrace{\nabla_B L(B; x_t, y_t)}_{\text{one example at a time}}$$

Why?

Where does these update rules come from?

Theory digest

Theory digest

- Fixed stepsize $\eta_t \equiv \eta \longrightarrow$ stable convergence
- Decreasing stepsize $\eta_t = \frac{\eta_0}{t+t_0} \longrightarrow$ faster local convergence, **with η_0 and t_0 properly set**
- Note: stochastic gradient descent is an *extreme* decomposition strategy picking *one example* at a time

In practice

- Pick a random batch of reasonable size, and find best pair (η_0, t_0) through cross-validation
- Run stochastic gradient descent with sequence of decreasing stepsize $\eta_t = \frac{\eta_0}{t+t_0}$

Tricks of the trades

Life is simpler in large-scale settings

- Shuffle the examples before launching the algorithm, and process the examples in a **balanced manner** w.r.t the categories
- Regularization through early stopping: perform only a few several passes/epochs over the training data, and stop when the accuracy on a held-out validation set does not increase anymore
- Fixed step-size works fine: find best η through cross-validation on a small batch

Stochastic gradient descent

Put the shoulder to the wheel

Let's try it out!

Ridge regression

Ridge regression

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$

$$\min_{\beta \in \mathbb{R}^d} \quad \frac{\lambda}{2}\|\beta\|_2^2 + \frac{1}{n}\sum_{i=1}^{n} L\left(y_i, \beta^T x_i\right)$$

Key calculations

$$Q\beta; x_i, y_i) := \frac{n\lambda}{2}\|\beta\|_2^2 + (y_i - \beta^T x_i)^2$$

$$\nabla Q(\beta; x_i, y_i) = n\lambda\beta + (y_i - \beta^T x_i)x$$

Logistic regression

Logistic regression

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$

$$\min_{\beta \in \mathbb{R}^d} \quad \frac{\lambda}{2}\|\beta\|_2^2 + \frac{1}{n}\sum_{i=1}^{n} L\left(y_i, \beta^T x_i\right)$$

Key calculations

$$Q(\beta; x_i, y_i) := \frac{n\lambda}{2}\|\beta\|_2^2 + \log\left(1 + \exp(-y_i \beta^T x_i)\right))$$

$$\nabla Q(\beta; x_i, y_i) = n\lambda\beta + -\frac{1}{1 + \exp(y_i \beta^T x_i)} y_i x_i$$

Linear SVM with linear hinge loss

Linear SVM with linear hinge loss

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$

$$\min_{\beta \in \mathbb{R}^d} \quad \frac{\lambda}{2}\|\beta\|_2^2 + \frac{1}{n}\sum_{i=1}^{n} L\left(y_i, \beta^T x_i\right)$$

Key calculations

$$Q(\beta; x_i, y_i) := \frac{n\lambda}{2}\|\beta\|_2^2 + \max\left(0, 1 - y_i \beta^T x_i\right)$$

$$\nabla Q(\beta; x_i, y_i) = \begin{cases} n\lambda\beta - y_i x_i & \text{if } 1 - y_i x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

Linear SVM with linear hinge loss

Linear SVM with linear hinge loss

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$

$$\min_{\beta \in \mathbb{R}^d} \quad \frac{\lambda}{2}\|\beta\|_2^2 + \frac{1}{n}\sum_{i=1}^{n} L\left(y_i, \beta^T x_i\right)$$

Non-differentiable loss

- Rule: if $L(\beta; x, y)$ has a finite number of a non-differentiable points, then just make **no update**, and pick another example.
- Theoretical justification: the set of a non-differentiable points will have measure zero, and convergence guarantee is still valid

A quick overview

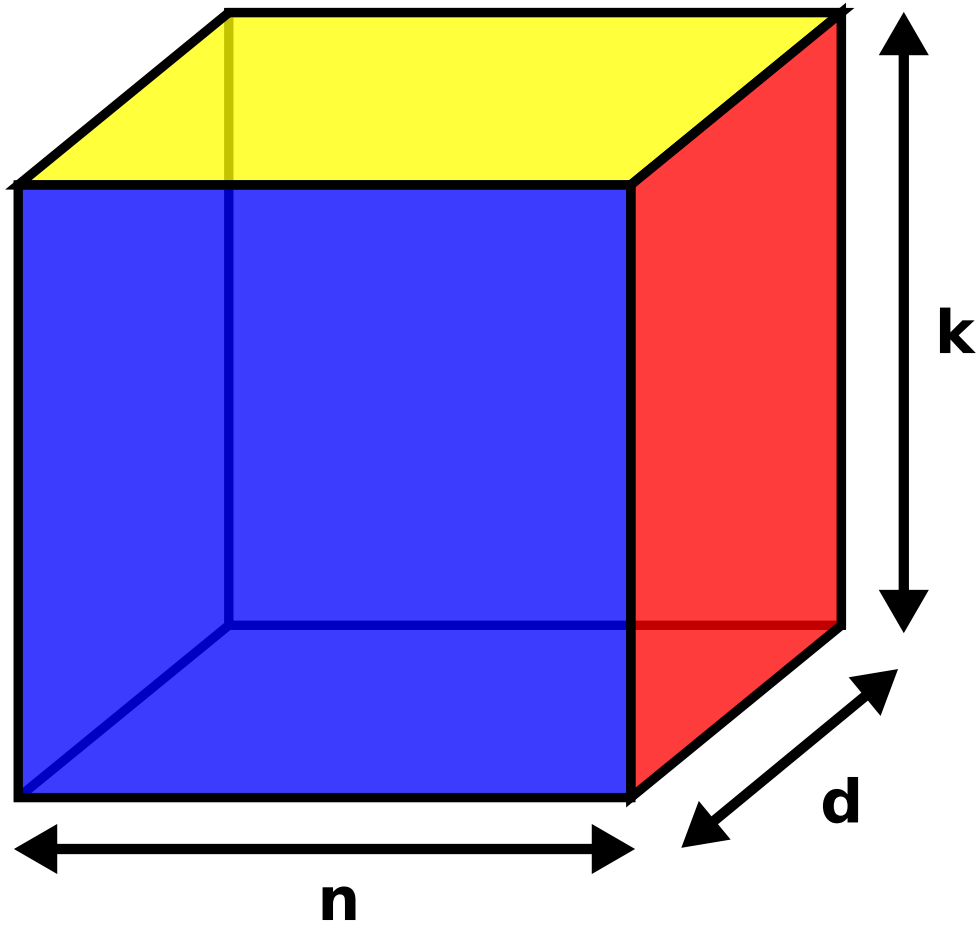
Convergence guarantees

- Least-square loss: smooth $\rightarrow$ fast and stable convergence
- Logistic loss: smooth $\rightarrow$ fast and stable convergence
- Linear hinge loss: non-smooth $\rightarrow$ slower convergence

Convergence guarantees

Take-home message: smooth loss is nicer

Machine learning cuboid



Decomposition principle

Decomposition principle

- Decomposition over examples: Stochastic gradient descent
- **Decomposition over categories: One-versus-rest strategy**
- Decomposition over features: Coordinate Descent
- Decomposition over set of image transformations: transformation pursuit

Multi-class linear SVM with regular linear hinge loss

Multi-class linear SVM with regular linear hinge loss

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \{0, 1\}^k$

$$\min_{B \in \mathbb{R}^{d \times k}} \quad \lambda \|\beta\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} \text{BinaryLogLoss}_i$$

One-versus-rest reduction

- Turn original label $y_i \in \{0, 1\}^k$ into binary label $\tilde{y}_i \in \{-1, +1\}$

$$\text{BinaryLogLoss}_i = \max(0, 1 - \tilde{y}_i \beta^T x_i)$$

- Note: any binary loss could do, i.e. also the **binary linear**

Multi-class linear SVM with regular linear hinge loss

Multi-class linear SVM with regular linear hinge loss

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \{0, 1\}^k$

$$\min_{\beta \in \mathbb{R}^{d \times k}} \quad \sum_{\ell=1}^{k} \lambda_\ell \left\| \beta_\ell \right\|_2^2 + \frac{1}{n} \sum_{\ell=1}^{k} \sum_{\substack{i=1 \\ y_i \equiv \text{class } \ell}}^{n} \text{BinaryLogLoss}_i$$

Decomposition over categories

Leverage **decomposable structure** over categories

Multi-class linear SVM with regular linear hinge loss

Multi-class linear SVM with regular linear hinge loss

Training data: $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^d \times \{0, 1\}^k$

$$
\begin{cases}
\min\limits_{\beta_1 \in \mathbb{R}^d} & \lambda_1 \left\|\beta_1\right\|_2^2 + \dfrac{1}{n} \sum\limits_{\substack{i=1 \\ y_i \equiv \text{class } 1}}^{n} \text{BinaryLogLoss}_i \\
\ldots & \\
\min\limits_{\beta_\ell \in \mathbb{R}^d} & \lambda_\ell \left\|\beta_\ell\right\|_2^2 + \dfrac{1}{n} \sum\limits_{\substack{i=1 \\ y_i \equiv \text{class } \ell}}^{n} \text{BinaryLogLoss}_i \\
\ldots & \\
\min\limits_{\beta_k \in \mathbb{R}^d} & \lambda_k \left\|\beta_k\right\|_2^2 + \dfrac{1}{n} \sum\limits_{\substack{i=1 \\ y_i \equiv \text{class } k}}^{n} \text{BinaryLogLoss}_i
\end{cases}
$$

Multi-class through one-vs-rest

Multi-class through one-vs-rest

- Overall: simplest multi-class classification algorithm
- Computational strength: easy to optimize by decomposition over classes
- Statistical weakness: no universally consistent loss can be decomposable over classes (do we really care? we'll see)

Multi-class through one-vs-rest

In practice

State-of-the-art performance using a **balanced** version of the binary loss, and **learning** the optimal imbalance β through cross-validation

$$\text{Empirical risk} = \frac{\beta}{n^+} \sum_{i \in \text{positive examples}} \text{BinaryLogLoss}_i + \frac{1-\beta}{n^-} \sum_{i \in \text{negative examples}} \text{BinaryLogLoss}_i$$

Multi-class with non-decomposable loss functions

Other multi-class loss functions

- Multinomial logistic loss
- Crammer & Singer multi-class loss

$$R_{\text{MUL}} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \max_{y} (\Delta(y_i, y) + \beta_y^T x_i) - \beta_{y_i}^T x_i \right\}$$

The multi-class binary hinge loss and the multi-class logistic loss are the only **decomposable** losses.

Multi-class with non-decomposable loss functions

More sophisticated losses

Loss functions tailored to optimize a nice surrogate to top-k accuracy

$$\text{Accuracy}_{\text{top}-k} = \frac{\#\text{ ex. with correct label lies in top-k scores}}{\text{Total number of ex.}}$$

- Ranking losses

$$R_{\text{RNK}} = \frac{1}{n}\sum_{i=1}^{n}\sum_{y=1}^{k}\max_{y}\left(0, \Delta(y_i, y) - (\beta_{y_i}^T - \beta_y)^T x_i\right)$$

- Weighted ranking losses, and other variations

Lasso Regression

Lasso Regression (Penalized Form)

The lasso regression solution for regularization parameter $\lambda \geq 0$ is

$$\hat{\beta} = \underset{\beta \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ \beta^T x_i - y_i \right\}^2 + \lambda \|\beta\|_1,$$

where $\|\beta\|_1 = |\beta_1| + \cdots + |\beta_d|$ is the ℓ_1-norm.

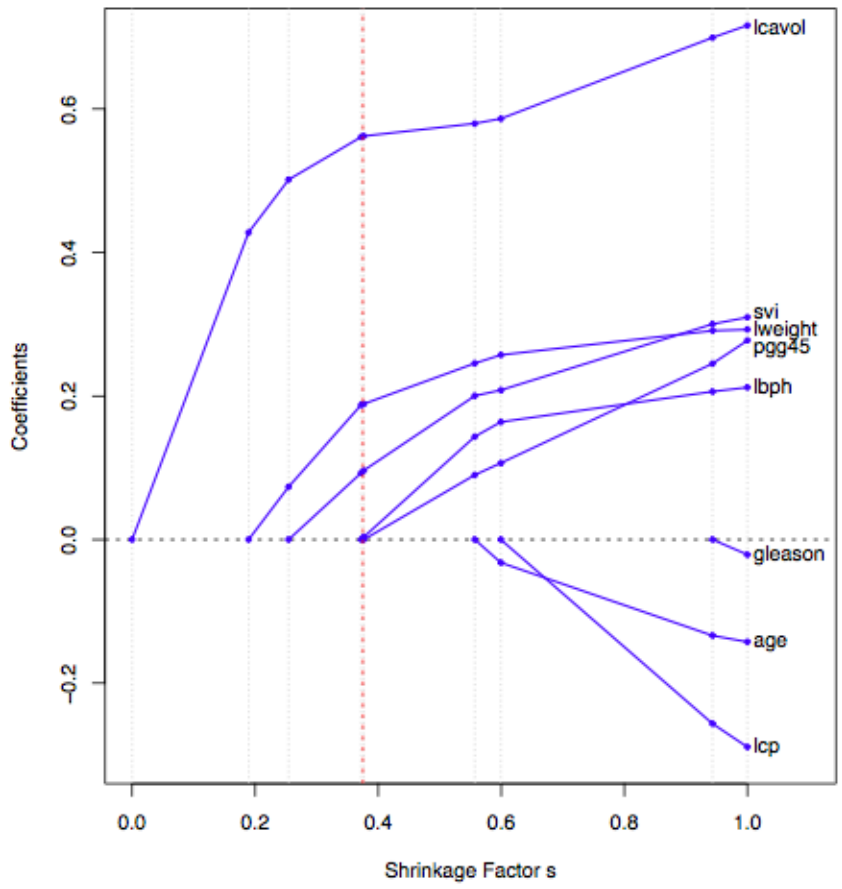
Lasso Regression

Lasso Regression (Constrained form)

The lasso regression solution for regularization parameter $r \geq 0$ is

$$\hat{\beta} = \underset{\|\beta\|_1 \leq r}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ \beta^T x_i - y_i \right\}^2 .$$

Lasso Regression: Regularization Path



Shrinkage Factor $s = r / \left|\hat{\beta}\right|_1$, where $\hat{\beta}$ is the ERM (the unpenalized fit).

Lasso Gives Feature Sparsity

- Time/expense to compute/buy features

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- Memory to store features (e.g. real-time deployment)

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Lasso Gives Feature Sparsity

- Time/expense to compute/buy features
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- Identifies the important features
- Better prediction? sometimes
- As a feature-selection step for training a slower non-linear model

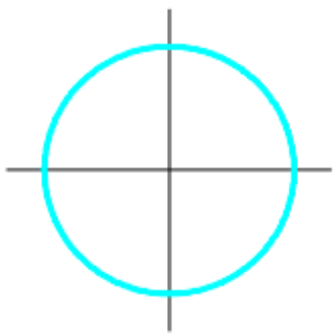
Constrained and Penalized Equivalent?

- For ridge regression and lasso regression,
  - the Constrained and Penalized formulations are equivalent
- We will use whichever form is most convenient.

The ℓ_1 and ℓ_2 Norm Constraints

- For visualization, restrict to 2-dimensional input space
- $\mathcal{F} = \{f(x) = \beta_1 x_1 + \beta_2 x_2\}$ (linear hypothesis space)
- Represent $\mathcal{F}$ by $\{(\beta_1, \beta_2) \in \mathbf{R}^2\}$.

- ℓ_2 contour: $\beta_1^2 + \beta_2^2 = r$



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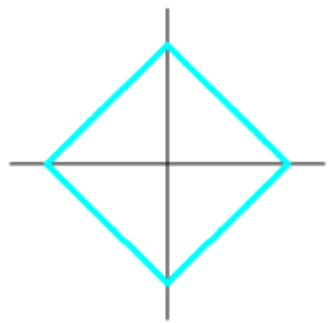

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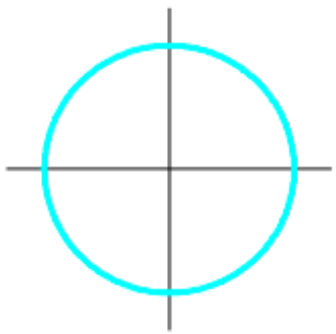

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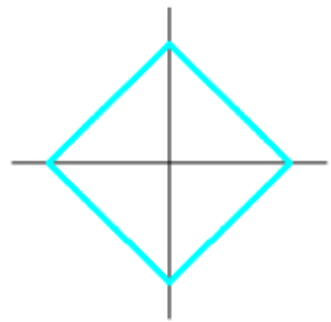
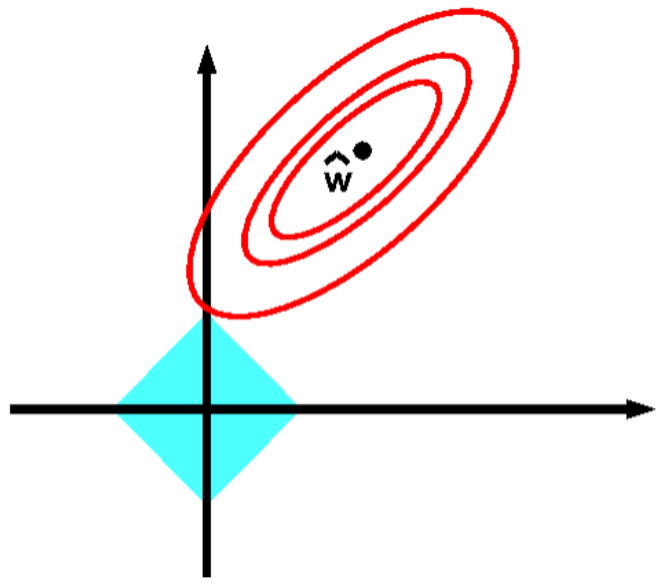


Where are the "sparse" solutions?

The Famous Picture for ℓ_1 Regularization

- $\min_r f_r =$
  $\arg\min_{\beta \in \mathbf{R}^2} \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2$ subject to $|\beta_1| + |\beta_2| \leq r$



- Red lines: contours of $\hat{R}_n(\beta) = \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2$.
- Blue region: Area satisfying complexity constraint:
  $|\beta_1| + |\beta_2| \leq r$

The Empirical Risk for Square Loss

- Denote the empirical risk of $f(x) = \beta^T x$ by

$$\hat{R}_n(\beta) = \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2 = \frac{1}{n} ||X\beta - y||^2$$

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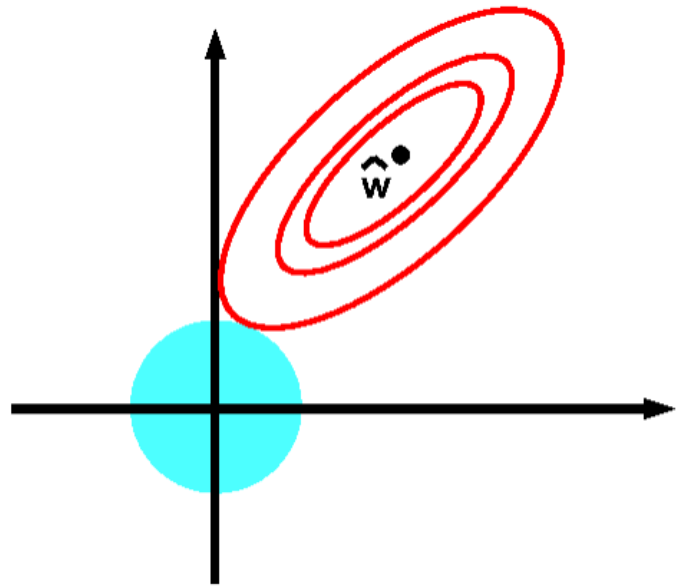
- $\hat{R}_n$ is minimized by the ordinary (un-regularized) least-squares solution.
- What does $\hat{R}_n$ look like around $\hat{\beta}$?

The Famous Picture for ℓ_2 Regularization

- $\min_r f_r =$
  $\arg\min_{\beta \in \mathbf{R}^2} \ \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2$ subject to $\beta_1^2 + \beta_2^2 \leq r$



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How to find the Lasso solution?

- How to solve the Lasso?

$$\min_{\beta \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2 + \lambda \left|\beta\right|_1$$

- $\left|\beta\right|_1$ is not differentiable!

Coordinate Descent Method

Coordinate Descent Method

Goal: Minimize $L(\beta) = L(\beta_1, \ldots \beta_d)$ over $\beta = (\beta_1, \ldots, \beta_d) \in \mathbf{R}^d$.

- **Initialize** $\beta^{(0)} = 0$
- **while** not converged:
  - Choose a coordinate $j \in \{1, \ldots, d\}$
  - $\beta_j^{\text{new}} \leftarrow \arg\min_{\beta_j} L(\beta_1^{(t)}, \ldots, \beta_{j-1}^{(t)}, \beta_{\mathbf{j}}, \beta_{j+1}^{(t)}, \ldots, \beta_d^{(t)})$
  - $\beta^{(t+1)} \leftarrow \beta^{(t)}$
  - $\beta_j^{(t+1)} \leftarrow \beta_j^{\text{new}}$
  - $t \leftarrow t + 1$

- **randomized coordinate descent**
- **cyclic coordinate descent**

Coordinate Descent Method for Lasso

- Why mention coordinate descent for Lasso?
- In Lasso, the coordinate minimization is **simple**.

Coordinate Descent Method for Lasso

Coordinate Minimization for Lasso

$$\hat{\beta}_j = \underset{\beta_j \in \mathbf{R}}{\arg\min} \; \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i \right)^2 + \lambda \left| \beta \right|_1$$

Coordinate Descent Method for Lasso

Coordinate Minimization for Lasso

$$\hat{\beta}_j = \arg\min_{\beta_j \in \mathbf{R}} \frac{1}{n} \sum_{i=1}^{n} \left(\beta^T x_i - y_i\right)^2 + \lambda \left|\beta\right|_1$$

Then

$$\hat{\beta}_j(c_j) = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

Coordinate Descent Method for Lasso

Coordinate Minimization for Lasso

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$$a_j = \frac{2}{n} \sum_{i=1}^{n} x_{i,j}^2 \qquad c_j = \frac{2}{n} \sum_{i=1}^{n} x_{i,j}(y_i - \beta_{-j}^T x_{i,-j})$$

where β_{-j} is β without component j and similarly for $x_{i,-j}$.

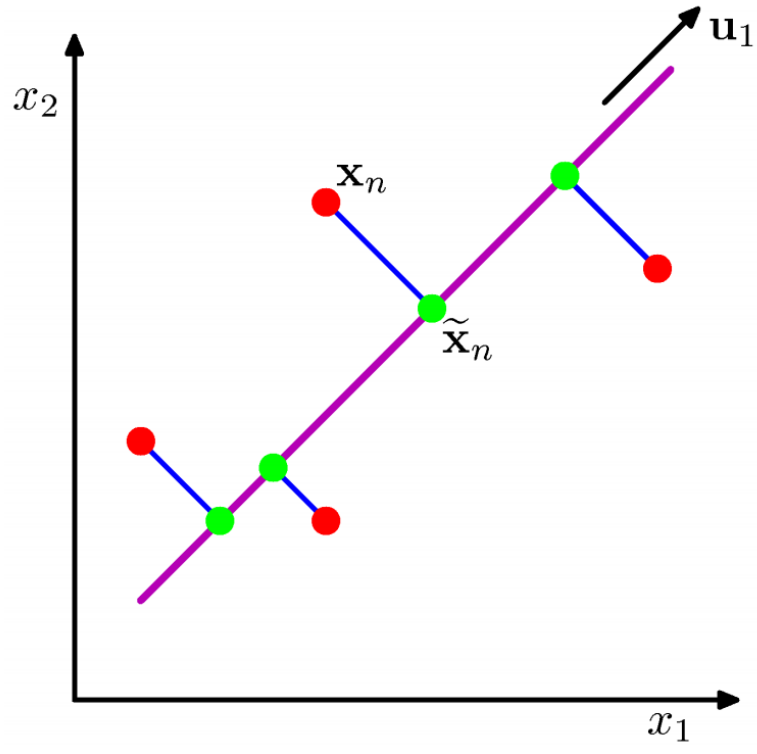
Coordinate Minimizer for Lasso

$$\hat{\beta}_j(c_j) = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

Dimension Reduction: Principal Component Analysis

Goal

- Project data onto a space with dimensional $M < D$
- Maximize the variance of the projected data



Principal Component Analysis

Goal:

- Maximum variance criterion corresponds to a Rayleigh quotient
- PCA boils down to an eigenvalue problem on the *centered* covariance matrix $\hat{\Sigma}$ of the dataset, that is the principal components $w_1, \ldots, w_d$ are the eigenvectors of $\hat{\Sigma}$ (assuming $n > d$)
- Computational complexity: $O(ndc)$ in time with a *Singular Value Decomposition* (SVD; see `eigs` in Matlab/Octave), with n the number of points, d the dimension, c the number of principal components retained; stochastic approximation version for nonstationary/large-scale datasets.

Principal Component Analysis

$$\text{Empirical mean} \quad \bar{x} = \frac{1}{N} \sum_{j=1}^{d} x_j$$

$$\text{Empirical covariance} \quad \hat{\Sigma} = \frac{1}{N} \sum_{j=1}^{d} (x_j - \bar{x})(x_j - \bar{x})^T$$

Projection along the direction w

- $\text{Proj}_w(x_j) = w^T x_j$, for all $j = 1, \ldots, N$
- $\text{Proj}_w(\bar{x}) = w^T \bar{x}$

Principal Component Analysis

Projection along the direction w

- $\text{Proj}_w(x_j) = w^T x_j$, for all $j = 1, \ldots, N$
- $\text{Proj}_w(\bar{x}) = w^T \bar{x}$

Variance of $\text{Proj}_w(x_j)$

$$\frac{1}{N} \sum_{j=1}^{N} (w^T x_j - w^T \bar{x})^2 = w^T \hat{\Sigma} w \ .$$

First Principal Component

Projection along the direction w

- $\text{Proj}_w(x_j) = w^T x_j$, for all $j = 1, \ldots, N$
- $\text{Proj}_w(\bar{x}) = w^T \bar{x}$

Variance of $\text{Proj}_w(x_j)$

$$\frac{1}{N} \sum_{j=1}^{N} (w^T x_j - w^T \bar{x})^2 = w^T \hat{\Sigma} w \ .$$

How to compute the top pair of eigenvalue and eigenvector: power iteration

For a matrix A, the Power Iteration algorithm returns the top pair of eigenvalue λ and eigenvector v of the matrix A.

Algorithm 1 Power Iteration Algorithm

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initialization v_0 random vector, and large number N .
repeat for $k = 1, 2, 3, \cdots, N$

- Perform update $z_k = Av_{k-1}$,
- Perform update $v_k = \frac{z_k}{\|z_k\|_2}, \lambda_k = v_k^T A v_k$.

until the stopping criterion is satisfied.

The Normalized Oja Algorithm

1. Pick randomly $w^{(0)}$ such that $\|w^{(0)}\|_2 = 1$.
2. Iterate
   - Update $w^{(t+1)} = w^{(t)} + \eta_t x_t x_t^T w^{(t)}$.
   - Normalize $w^{(t+1)} = \frac{w^{(t+1)}}{\|w^{(t+1)}\|_2}$.

Variance along a direction and Rayleigh quotients

PCA seeks for directions $w_1, \ldots, w_c$ such that

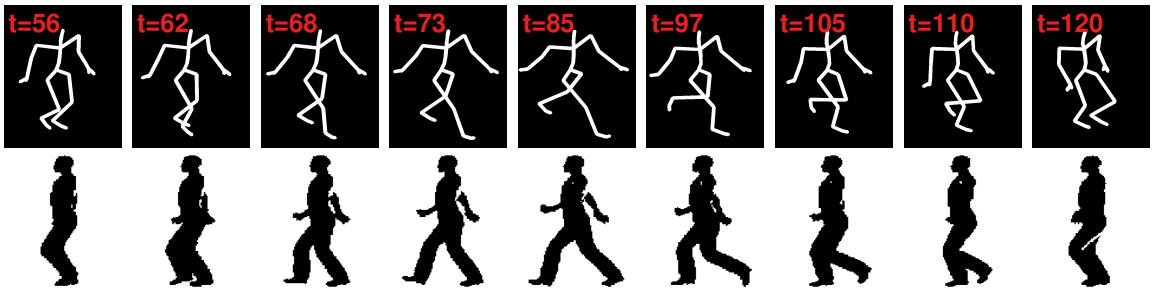
$$
\begin{aligned}
w_j &= \text{argmax}_{w \in \mathbb{R}^d; w_j \perp \{w_1, \ldots, w_{j-1}\}} \text{Var}_x \left\{ \frac{w^T x}{w^T w} \right\} \\
&= \text{argmax}_{w \in \mathbb{R}^d; w_j \perp \{w_1, \ldots, w_{j-1}\}} \frac{1}{m} \sum_{i=1}^{m} \frac{(w^T x_i)^2}{w^T w} \\
&= \text{argmax}_{w \in \mathbb{R}^d; w_j \perp \{w_1, \ldots, w_{j-1}\}} \underbrace{\frac{w^T \hat{\Sigma} w}{w^T w}}_{\text{Rayleigh quotient}} .
\end{aligned}
$$

Principal components $w_1, \ldots, w_c$ are the first c eigenvectors of $\hat{\Sigma}$.

Low-dimensional representation with PCA

- Walking sequence of length 400 (containing about 3 walking cycles) obtained from the CMU Mocap database
- Data: silhouette images taken at a side view

Human body pose representation (Kim & Pavlovic, 2008). Selected skeleton and silhouette images for a half walking cycle.



Low-dimensional representation with PCA

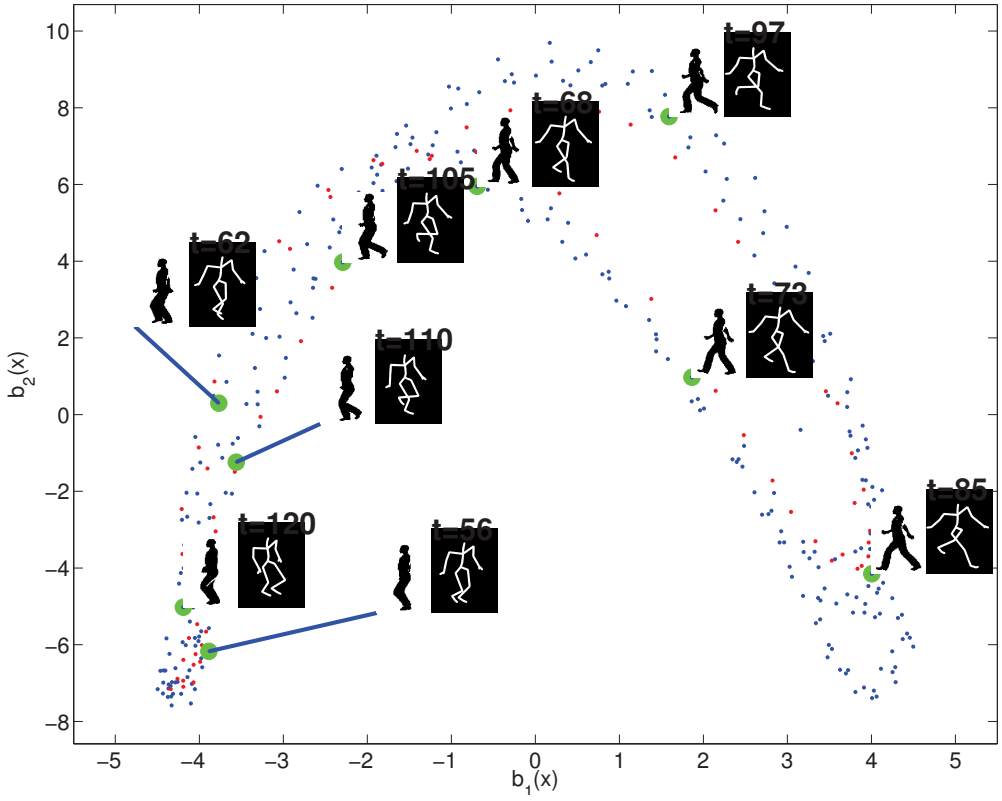


Figure: Central subspaces for silhouette images from walking motion

Low-dimensional representation with PCA

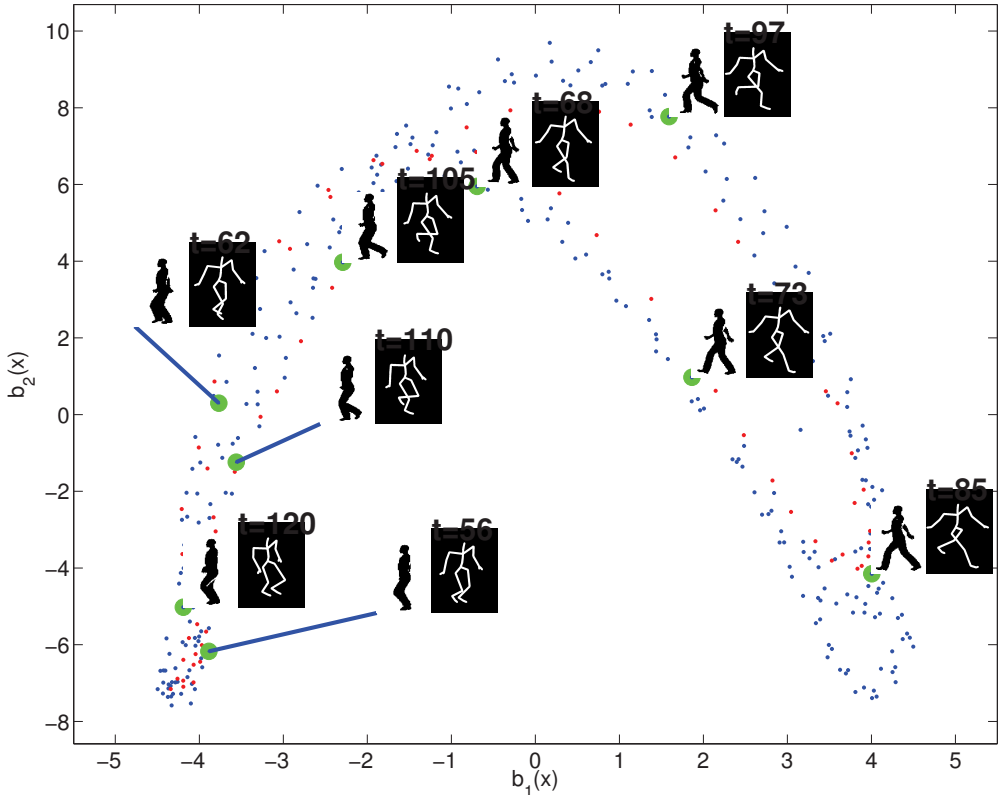


Figure: Central subspaces for silhouette images from walking motion

Super-resolution with PCA (Kim et al., 2005)

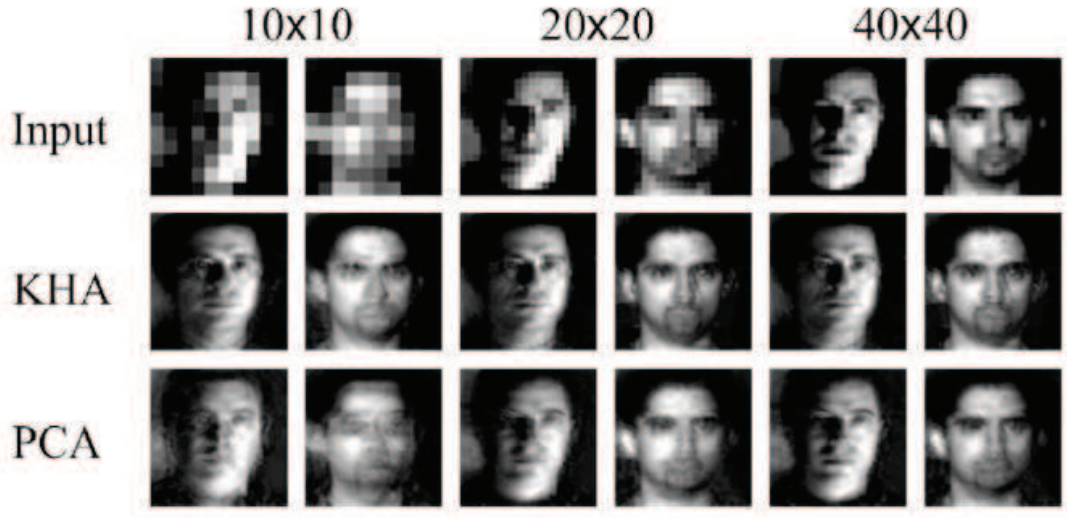


Figure: Super-resolution from low-resolution images of faces

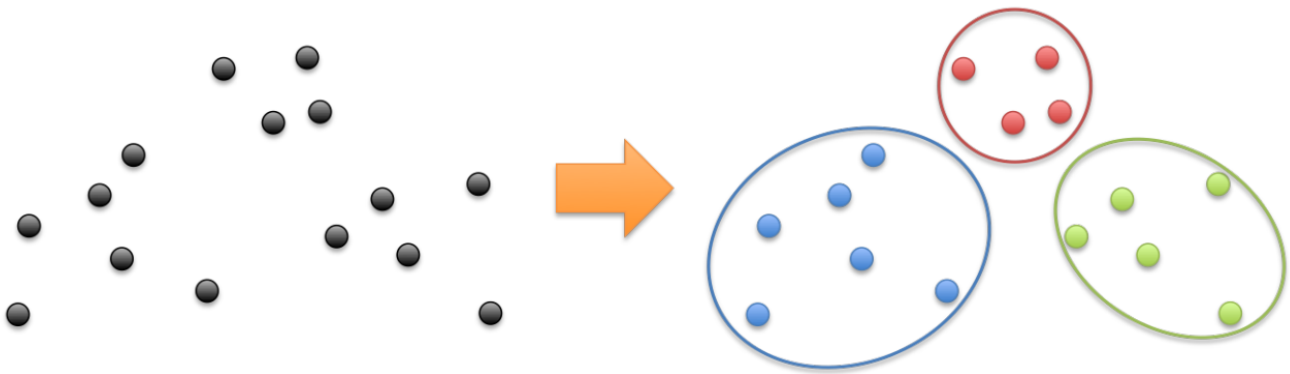
Applications

- Image denoising (digits, faces, etc.)
- Visualization of bioinformatics data (strings, proteins, etc.)
- Dimension-reduction of high-dimensional features (appearance, interest points, etc.)

Clustering

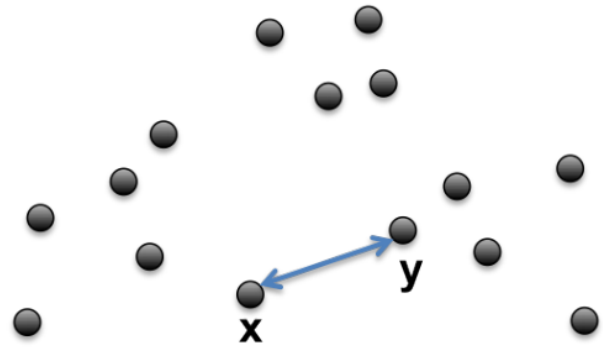
Goal is to group "similar" instances together.

- Given data points $x_i \in \mathbf{R}^d$, $i = 1, \ldots, n$.
- But no labels unsupervised learning
- Useful for exploratory data analysis



Clustering

Need measure of similarity (or distance) between x and y.



Popular distance metrics:

- Squared Euclidean distance $d(x, y) = \|x - y\|_2^2$
- Cosine similarity $d(x, y) = (x^T y)/(\|x\|\|y\|)$
- Manhattan distance $d(x, y) = \|x - y\|_1$

Clustering results are crucially dependent on the distance metric.

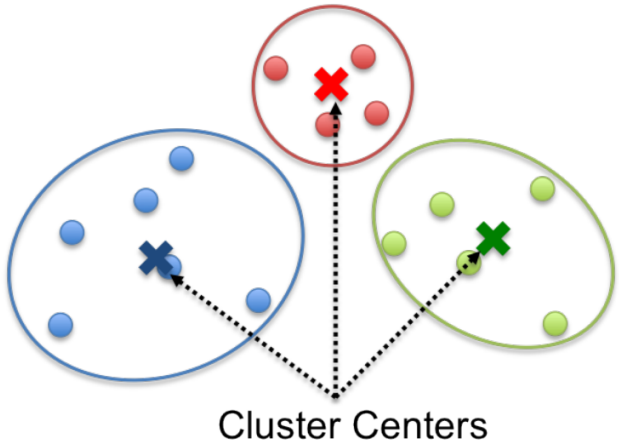
Clustering

Find k clusters that minimizes the objective:

$$J = \sum_{i=1}^{k} \sum_{x \in \mathcal{C}_i} \|x - m_i\|_2^2$$

where

- $\mathcal{C}_i$ set of points in cluster i
- m_i mean of cluster i
- Objective is non-convex and problem is NP-hard in general



Unsupervised Learning: Clustering

Input: data points $\boldsymbol{x} \in \mathbb{R}^d$, number of clusters k
Output: cluster assignment $\mathcal{C}_i$ of data points, $i = 1, 2, \ldots, k$

1: Randomly partition the data into k clusters
2: **while** not converged **do**
3: Compute mean of each cluster i

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\boldsymbol{x} \in \mathcal{C}_i} \boldsymbol{x}$$

4: For each $\boldsymbol{x}$, find its new cluster index:

$$\pi(\boldsymbol{x}) = \arg \min_{1 \le i \le k} \|\boldsymbol{x} - \mathbf{m}_i\|_2^2$$

5: Update clusters:

$$\mathcal{C}_i = \{\boldsymbol{x} | \pi(\boldsymbol{x}) = i\}$$

6: **end while**

Clustering

Let the objective at the t-th iteration be

$$J^{(t)} = \sum_{i=1}^{k} \sum_{x \in \mathcal{C}_i^{(t)}} \|x - m_i^{(t)}\|_2^2 .$$

We have

$$\begin{aligned} J^{(t)} &\geq \sum_{i=1}^{k} \sum_{x \in \mathcal{C}_i^{(t)}} \|x - m_{\pi(x)}^{(t)}\|_2^2 \\ &= \sum_{i=1}^{k} \sum_{x \in \mathcal{C}_{i+1}^{(t)}} \|x - m_i^{(t)}\|_2^2 \\ &\geq \sum_{i=1}^{k} \sum_{x \in \mathcal{C}_{i+1}^{(t)}} \|x - m_i^{(t+1)}\|_2^2 \\ &= J^{(t+1)} \end{aligned}$$

Clustering

- Each step decreases the objective - convergence guarantee
- Convergence to a stationary point, not necessarily the global minimum

Clustering

Input: data points $\boldsymbol{x} \in \mathbb{R}^d$, number of clusters k
Output: cluster assignment $\mathcal{C}_i$ of data points, $i = 1, 2, \ldots, k$

1: Initialize means $\mathbf{m}_i$ and $n_i = 0$, $i = 1, 2, \ldots, k$
2: **while** not converged **do**
3: Pick a data point $\boldsymbol{x}$ and determine cluster $\pi(\boldsymbol{x})$

$$\pi(\boldsymbol{x}) = \arg \min_{1 \leq i \leq k} \|\boldsymbol{x} - \mathbf{m}_i\|_2^2$$

4: Update mean $\mathbf{m}_{\pi(\boldsymbol{x})}$

$$n_{\pi(\boldsymbol{x})} = n_{\pi(\boldsymbol{x})} + 1 \quad \text{and} \quad \mathbf{m}_{\pi(\boldsymbol{x})} = \mathbf{m}_{\pi(\boldsymbol{x})} + \frac{1}{n_{\pi(\boldsymbol{x})}}(\boldsymbol{x} - \mathbf{m}_{\pi(\boldsymbol{x})})$$

5: **end while**