Lecture 7: Kernels for Classification and Regression

CS 194-10, Fall 2011

Laurent El Ghaoui

EECS Department
UC Berkeley

September 15, 2011

Outline

Outline

A linear regression problem

Linear auto-regressive model for time-series: y_t linear function of y_{t-1}, y_{t-2}

$$y_t = w_1 + w_2 y_{t-1} + w_3 y_{t-2}, \quad t = 1, \ldots, T.$$

This writes $y_t = w^T x_t$, with x_t the "feature vectors"

$$x_t := (1, y_{t-1}, y_{t-2}), \quad t = 1, \ldots, T.$$

Model fitting via least-squares:

$$\min_w \ \|X^T w - y\|_2^2$$

Prediction rule : $\hat{y}_{T+1} = w_1 + w_2 y_T + w_3 y_{T-1} = w^T x_{T+1}$.

Nonlinear regression

Nonlinear auto-regressive model for time-series: y_t quadratic function of y_{t-1}, y_{t-2}

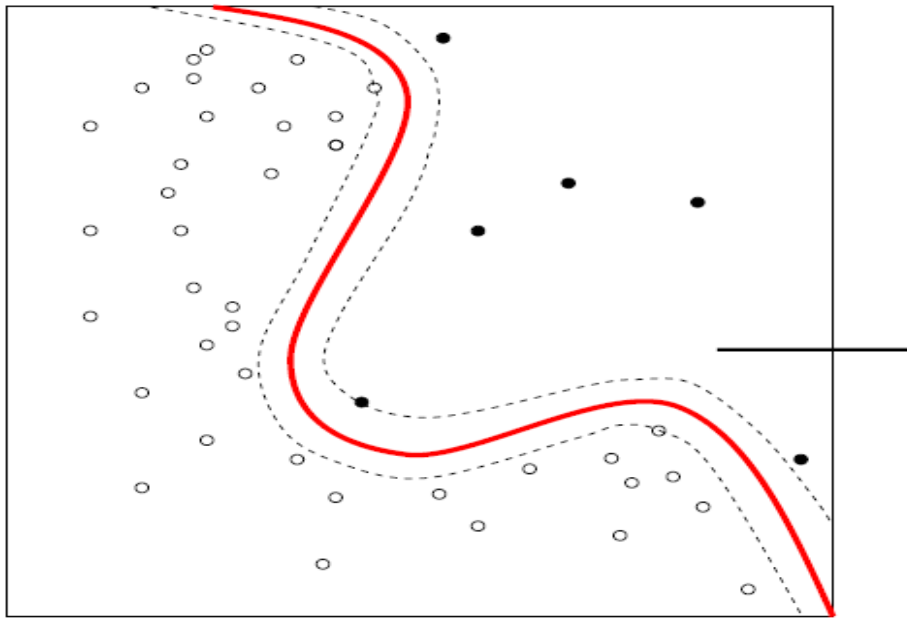
$$y_t = w_1 + w_2 y_{t-1} + w_3 y_{t-2} + w_4 y_{t-1}^2 + w_5 y_{t-1} y_{t-2} + w_6 y_{t-2}^2.$$

This writes $y_t = w^T \phi(x_t)$, with $\phi(x_t)$ the augmented feature vectors

$$\phi(x_t) := \left(1, y_{t-1}, y_{t-2}, y_{t-1}^2, y_{t-1} y_{t-2}, y_{t-2}^2\right).$$

Everything the same as before, with x replaced by $\phi(x)$.

Nonlinear classification



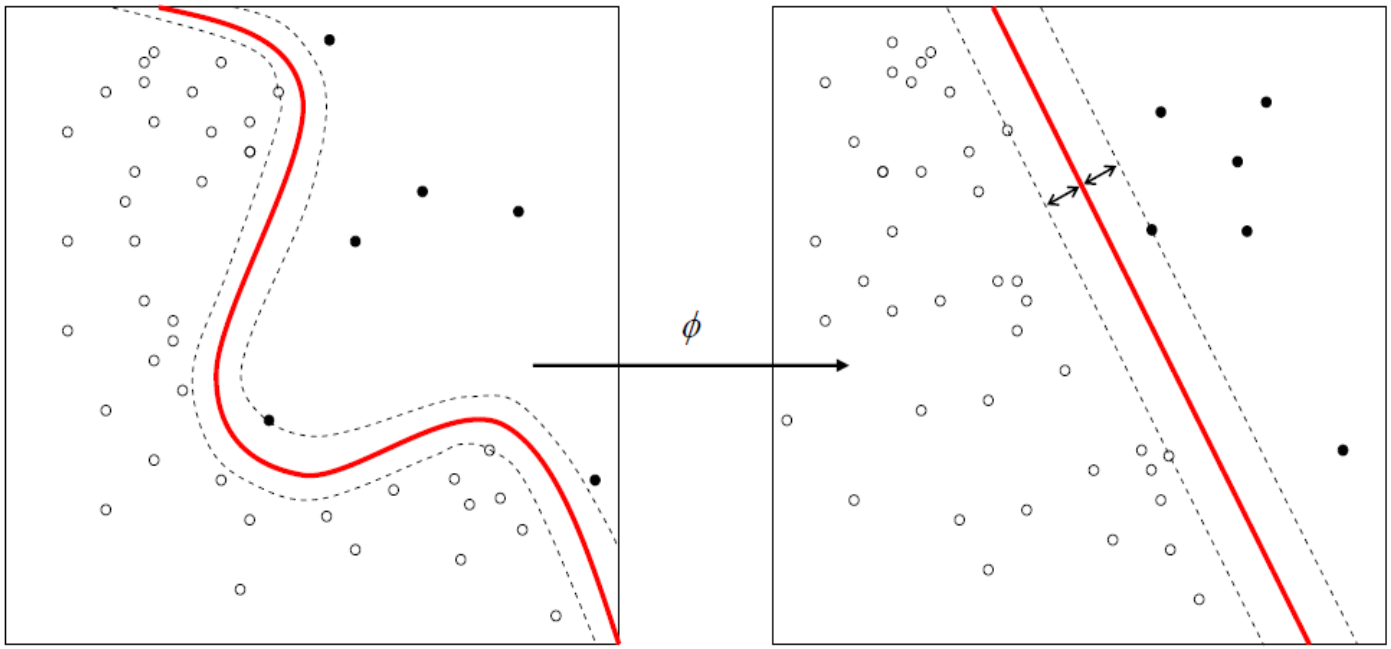
Non-linear (*e.g.*, quadratic) decision boundary

$$w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_1 x_2 + w_5 x_2^2 + b = 0.$$

Writes $w^T \phi(x) + b = 0$, with $\phi(x) := (x_1, x_2, x_1^2, x_1 x_2, x_2^2)$.

Challenges

In principle, it seems can always augment the dimension of the feature space to make the data linearly separable. (See the video at http://www.youtube.com/watch?v=3liCbRZPrZA)



How do we do it in a computationally efficient manner?

Outline

Linear least-squares

$$\min_w \ \|X^T w - y\|_2^2 + \lambda \|w\|_2^2$$

where

- $X = [x_1, \ldots, x_n]$ is the $m \times n$ matrix of data points.
- $y \in \mathbf{R}^m$ is the "response" vector,
- w contains regression coefficients.
- $\lambda \geq 0$ is a regularization parameter.

Prediction rule: $y = w^T x$, where $x \in \mathbf{R}^n$ is a new data point.

Support vector machine (SVM)

$$\min_w \sum_{i=1}^{m} (1 - y_i(w^T x_i + b)) + \lambda \|w\|_2^2$$

where

- $X = [x_1, \ldots, x_m]$ is the $n \times m$ matrix of data points in $\mathbf{R}^n$.
- $y \in \{-1, 1\}^m$ is the label vector.
- w, b contain classifer coefficients.
- $\lambda \geq 0$ is a regularization parameter.

In the sequel, we'll ignore the bias term (for simplicity only).

Classification rule: $y = \mathbf{sign}(w^T x + b)$, where $x \in \mathbf{R}^n$ is a new data point.

Generic form of problem

Many classification and regression problems can be written

$$\min_w \; L(X^T w, y) + \lambda \|w\|_2^2$$

where

- $X = [x_1, \ldots, x_n]$ is a $m \times n$ matrix of data points.
- $y \in \mathbf{R}^m$ contains a response vector (or labels).
- w contains classifier coefficients.
- L is a "loss" function that depends on the problem considered.
- $\lambda \geq 0$ is a regularization parameter.

Prediction/classification rule: depends only on $w^T x$, where $x \in \mathbf{R}^n$ is a new data point.

Loss functions

- Squared loss: (for linear least-squares regression)

$$L(z, y) = \|z - y\|_2^2.$$

- Hinge loss: (for SVMs)

$$L(z, y) = \sum_{i=1}^{m} \max(0, 1 - y_i z_i)$$

- Logistic loss: (for logistic regression)

$$L(z, y) = -\sum_{i=1}^{m} \log(1 + e^{-y_i z_i}).$$

Outline

Key result

For the generic problem:

$$\min_w \; L(X^T w) + \lambda \|w\|_2^2$$

the optimal w lies in the span of the data points $(x_1, \ldots, x_m)$:

$$w = Xv$$

for some vector $v \in \mathbf{R}^m$.

Proof

Any $w \in \mathbf{R}^n$ can be written as the sum of two *orthogonal* vectors:

$$w = Xv + r$$

where $X^T r = 0$ (that is, r is in the nullspace $\mathcal{N}(X^T)$).

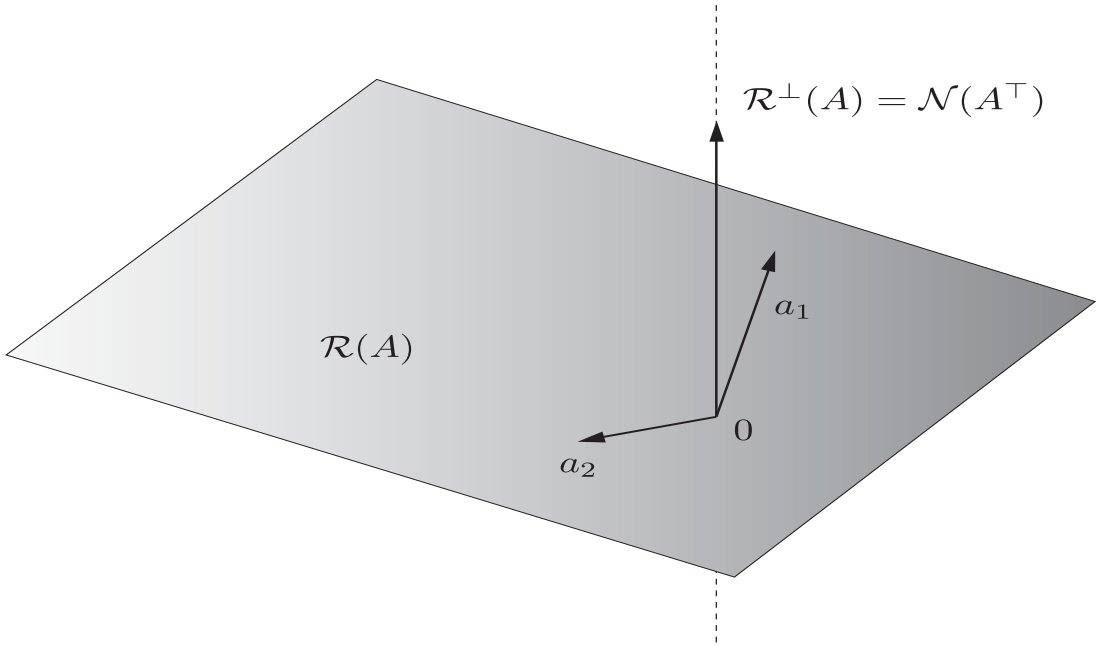


Figure shows the case $X = A = (a_1, a_2)$.

Consequence of key result

For the generic problem:

$$\min_w \; L(X^T w) + \lambda \|w\|_2^2$$

the optimal w can be written as $w = Xv$ for some vector $v \in \mathbf{R}^m$.

Hence training problem depends only on $K := X^T X$:

$$\min_v \; L(Kv) + \lambda v^T K v.$$

Kernel matrix

The training problem depends only on the "kernel matrix" $K = X^T X$

$$K_{ij} = x_i^T x_j$$

K contains the scalar products between all data point pairs.

The prediction/classification rule depends on the scalar products between new point x and the data points $x_1, \ldots, x_m$:

$$w^T x = v^T X^T x = v^T k, \quad k := X^T x = (x^T x_1, \ldots, x^T x_m).$$

Computational advantages

Once K is formed (this takes $O(n)$), then the training problem has only m variables.

When $n >> m$, this leads to a dramatic reduction in problem size.

How about the nonlinear case?

In the nonlinear case, we simply replace the feature vectors x_i by some "augmented" feature vectors $\phi(x_i)$, with ϕ a non-linear mapping.

Example : in classification with quadratic decision boundary, we use

$$\phi(x) := (x_1, x_2, x_1^2, x_1 x_2, x_2^2).$$

This leads to the modified kernel matrix

$$K_{ij} = \phi(x_i)^T \phi(x_j), \quad 1 \leq i, j \leq m.$$

The kernel function

The kernel function associated with mapping ϕ is

$$k(x, z) = \phi(x)^T \phi(z).$$

It provides information about the metric in the feature space, *e.g.*:

$$\|\phi(x) - \phi(z)\|_2^2 = k(x, x) - 2k(x, z) + k(z, z).$$

The computational effort involved in

- solving the training problem;
- making a prediction,

depends only on our ability to quickly evaluate such scalar products.

We can't choose k arbitrarily; it has to satisfy the above for some ϕ.

Outline

Quadratic kernels

Classification with quadratic boundaries involves feature vectors

$$\phi(x) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2).$$

Fact : given two vectors $x, z \in \mathbf{R}^2$, we have

$$\phi(x)^T \phi(z) = (1 + x^T z)^2.$$

Polynomial kernels

More generally when $\phi(x)$ is the vector formed with all the products between the components of $x \in \mathbf{R}^n$, up to degree d, then for any two vectors $x, z \in \mathbf{R}^n$,

$$\phi(x)^T \phi(z) = (1 + x^T z)^d.$$

Computational effort grows linearly in n.

This represents a dramatic reduction in speed over the "brute force" approach:

- Form $\phi(x)$, $\phi(z)$;
- evaluate $\phi(x)^T \phi(z)$.

Computational effort grows as n^d.

Other kernels

Gaussian kernel function:

$$k(x, z) = \exp\left(-\frac{\|x - z\|_2^2}{2\sigma^2}\right),$$

where $\sigma > 0$ is a scale parameter. Allows to ignore points that are too far apart. Corresponds to a non-linear mapping ϕ to infinite-dimensional feature space.

There is a large variety (a zoo?) of other kernels, some adapted to structure of data (text, images, etc).

In practice

- Kernels need to be chosen by the user.
- Choice not always obvious; Gaussian or polynomial kernels are popular.
- Control over-fitting via cross validation (wrt say, scale parameter of Gaussian kernel, or degree of polynomial kernel).
- Kernel methods not well adapted to l_1-norm regularization.