6 - Regression problems

G. Mastroeni and M. Passacantando

Department of Computer Science, University of Pisa

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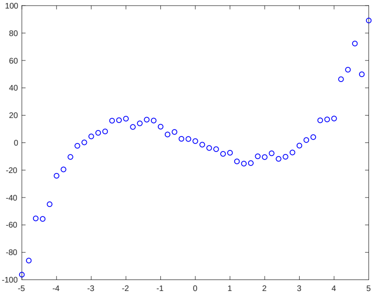
Polynomial regression

We have ℓ experimental data $y_1, y_2, \dots, y_\ell \in \mathbb{R}$ corresponding to the observations related to the points $x_1, x_2, \dots, x_\ell \in \mathbb{R}$.



We want to find the best approximation of experimental data with a polynomial p of degree $n-1$, with $n \leq \ell$.
Polynomial p has coefficients $z_1, \dots, z_n$:

$$p(x) = z_1 + z_2\,x + z_3\,x^2 + \cdots + z_n\,x^{n-1}$$

The residual is the vector $r \in \mathbb{R}^\ell$ such that $r_i = p(x_i) - y_i$, with $i = 1, \dots, \ell$.

We want to find coefficients $z := (z_1, z_2, .., z_n)$ of polynomial p such that $\|r\|$ is minimum, which amounts to solve the following unconstrained problem

$$\begin{cases} \min \ \|A\,z - y\| \\ z \in \mathbb{R}^n \end{cases}$$

where

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_\ell & x_\ell^2 & \dots & x_\ell^{n-1} \end{pmatrix} \in \mathbb{R}^{\ell \times n} \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_\ell \end{pmatrix}$$

For any norm, the objective function $f(z) = \|Az - y\|$ is convex.

We will consider three special norms: $\|\cdot\|_2$, $\|\cdot\|_1$ and $\|\cdot\|_\infty$.

Polynomial regression with $\|\cdot\|_2$

Euclidean norm $\|\cdot\|_2$ (least squares approximation)
$\rightarrow$ unconstrained quadratic programming problem:

$$\begin{cases} \min \ \frac{1}{2}\|Az - y\|_2^2 = \frac{1}{2}(Az-y)^{\mathsf{T}}(Az-y) = \frac{1}{2}z^{\mathsf{T}}A^{\mathsf{T}}Az - z^{\mathsf{T}}A^{\mathsf{T}}y + \frac{1}{2}y^{\mathsf{T}}y \\ z \in \mathbb{R}^n \end{cases}$$

It can be proved that $\operatorname{rank}(A) = n$, thus $A^{\mathsf{T}}A$ is positive definite.

Hence, the unique optimal solution is the stationary point of the objective function, i.e., the solution of the system of linear equations:

$$A^{\mathsf{T}}Az = A^{\mathsf{T}}y \tag{1}$$

Polynomial regression with $\|\cdot\|_1$

Norm $\|\cdot\|_1$ $\rightarrow$ linear programming problem:

$$\begin{cases} \min \ \|Az - y\|_1 = \min \ \sum_{i=1}^{\ell} |A_i z - y_i| \\ z \in \mathbb{R}^n \end{cases}$$

is equivalent to

$$\begin{cases} \min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\ u_i = |A_i z - y_i| \\ \quad = \max\{A_i z - y_i, y_i - A_i z\} \end{cases} \rightarrow \begin{cases} \min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\ u_i \geq \max\{A_i z - y_i, y_i - A_i z\} \end{cases}$$

$$\rightarrow \begin{cases} \min\limits_{z,u} \ \sum_{i=1}^{\ell} u_i \\ u_i \geq A_i z - y_i & \forall \ i = 1, \dots, \ell \\ u_i \geq y_i - A_i z & \forall \ i = 1, \dots, \ell \end{cases} \tag{2}$$

In matrix form (2) can be written as

$$\begin{cases} \min\limits_{z,u} \ e_\ell^T u \\ Az - u \leq y \\ -Az - u \leq -y \end{cases}$$

where $e^T = (1, ..., 1) \in \mathbb{R}^\ell$.
Set

$$D = \begin{pmatrix} A & -I_\ell \\ -A & -I_\ell \end{pmatrix} \quad d = \begin{pmatrix} y \\ -y \end{pmatrix}$$

where I_ℓ is the identity matrix of order ℓ, then we obtain

$$\begin{cases} \min\limits_{z,u} \ (0_n^T, e_\ell^T) \begin{pmatrix} z \\ u \end{pmatrix} \\ D \begin{pmatrix} z \\ u \end{pmatrix} \leq d \end{cases}$$

Norm $\|\cdot\|_\infty \to$ linear programming problem:

$$\begin{cases} \min \ \|Az - y\|_\infty = \min \ \max\limits_{i=1,\dots,\ell} |A_i z - y_i| \\ z \in \mathbb{R}^n \end{cases}$$

is equivalent to

$$\begin{cases} \min\limits_{z,u} \ u \\ u = \max\limits_{i=1,\dots,\ell} |A_i z - y_i| \end{cases} \to \begin{cases} \min\limits_{z,u} \ u \\ u \geq A_i z - y_i & \forall \ i = 1, \dots, \ell \\ u \geq y_i - A_i z & \forall \ i = 1, \dots, \ell \end{cases} \tag{3}$$

Set

$$D = \begin{pmatrix} A & -e_\ell \\ -A & -e_\ell \end{pmatrix} \quad d = \begin{pmatrix} y \\ -y \end{pmatrix}$$

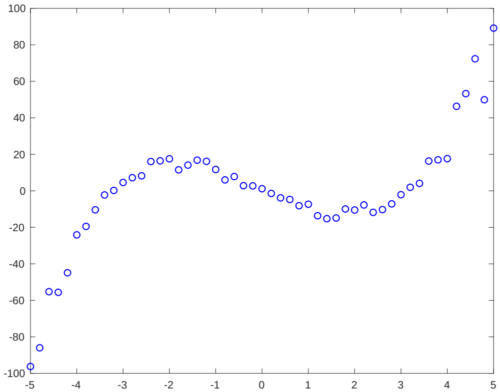
where $e_\ell = (1, \dots, 1) \in \mathbb{R}^\ell$, in matrix form (3) becomes:

$$\begin{cases} \min\limits_{z,u} \ (0, 0, \dots, 0, 1) \begin{pmatrix} z \\ u \end{pmatrix} \\ D \begin{pmatrix} z \\ u \end{pmatrix} \leq d \end{cases}$$

Exercise 6.1. Consider the experimental data (x_i, y_i), $i = 1, .., \ell$, given below:

$$\begin{pmatrix} -5.0000 & -96.2607 \\ -4.8000 & -85.9893 \\ -4.6000 & -55.2451 \\ -4.4000 & -55.6153 \\ -4.2000 & -44.8827 \\ -4.0000 & -24.1306 \\ -3.8000 & -19.4970 \\ -3.6000 & -10.3972 \\ -3.4000 & -2.2633 \\ -3.2000 & 0.2196 \\ -3.0000 & 4.5852 \\ -2.8000 & 7.1974 \\ -2.6000 & 8.2207 \\ -2.4000 & 16.0614 \\ -2.2000 & 16.4224 \\ -2.0000 & 17.5381 \\ -1.8000 & 11.4895 \\ -1.6000 & 14.1065 \\ -1.4000 & 16.8220 \\ -1.2000 & 16.1584 \\ -1.0000 & 11.6846 \\ -0.8000 & 5.9991 \\ -0.6000 & 7.8277 \\ -0.4000 & 2.8236 \\ -0.2000 & 2.7129 \\ 0 & 1.1669 \end{pmatrix} \qquad \begin{pmatrix} 0.2000 & -1.4223 \\ 0.4000 & -3.8489 \\ 0.6000 & -4.7101 \\ 0.8000 & -8.1538 \\ 1.0000 & -7.3364 \\ 1.2000 & -13.6464 \\ 1.4000 & -15.2607 \\ 1.6000 & -14.8747 \\ 1.8000 & -9.9271 \\ 2.0000 & -10.5022 \\ 2.2000 & -7.7297 \\ 2.4000 & -11.7859 \\ 2.6000 & -10.2662 \\ 2.8000 & -7.1364 \\ 3.0000 & -2.1166 \\ 3.2000 & 1.9428 \\ 3.4000 & 4.0905 \\ 3.6000 & 16.3151 \\ 3.8000 & 16.9854 \\ 4.0000 & 17.6418 \\ 4.2000 & 46.3117 \\ 4.4000 & 53.2609 \\ 4.6000 & 72.3538 \\ 4.8000 & 49.9166 \\ 5.0000 & 89.1652 \end{pmatrix}$$

Find the best approximating polynomials of degree 3 with respect to the norms $\| \cdot \|_2$, $\| \cdot \|_1$, $\| \cdot \|_\infty$.



- For the case of norm $\|\cdot\|_2$, the solution is given by (1).
- For the cases of norms $\|\cdot\|_2$, $\|\cdot\|_1$, $\|\cdot\|_\infty$, we have to solve problems (2) and (3) written in matrix form.

We will use the Matlab function "linprog".

From the Matlab help

- X = linprog(f,A,b) attempts to solve the linear programming problem:

$$\min_x f' * x \text{ subject to: } A * x <= b$$

- X = linprog(f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints $Aeq * x = beq$.
  (Set A=[] and B=[] if no inequalities exist.)
- X = linprog(f,A,b,Aeq,beq,LB,UB) defines a set of lower and upper bounds on the design variables, X, so that the solution is in the range LB <= X <= UB. Use empty matrices for LB and UB if no bounds exist. Set LB(i) = -Inf if X(i) is unbounded below; set UB(i) = Inf if X(i) is unbounded above.

Exercise 6.1: Matlab commands

```
data =[....];              %Matrix of given data

x = data(:,1) ;
y = data(:,2) ;
l = length(x) ;
n = 4 ;                          % number of coefficients of polynomial
A = [ ones(l,1) x x.^ 2 x.^ 3 ];    % Vandermonde matrix
```

% 2-norm problem

```
z2 = inv(A'*A)*(A'*y)
p2 = A*z2;               % regression values at the data
```

% 1-norm problem

```
c = [ zeros(n,1); ones(l,1) ];
D = [ A -eye(l); -A -eye(l) ];
d = [ y; -y ];
sol1 = linprog(c,D,d) ;
z1 = sol1(1:n)
p1 = A*z1;               % regression values at the data
```

% inf-norm problem

```
c = [ zeros(n,1); 1 ];
D = [ A -ones(l,1); -A -ones(l,1) ];
solinf = linprog(c,D,d) ;
zinf = solinf(1:n)
pinf = A*zinf;               % regression values at the data
```

% plot the solutions

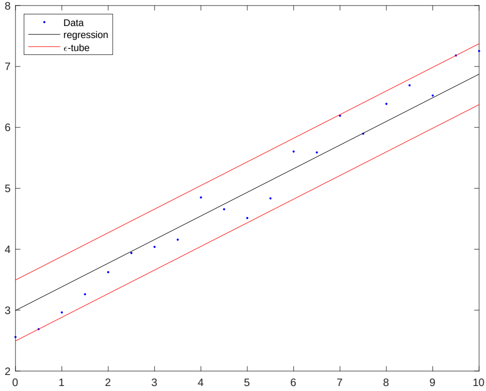
```
plot(x,y,'b.',x,p2,'r-',x,p1,'k-',x,pinf,'g-')
legend('Data','2-norm','1-norm','inf-norm','Location','NorthWest');
```

ε-SV regression

Given a set of training data $\{(x_1, y_1), \ldots, (x_\ell, y_\ell)\}$, where $x_i \in \mathbb{R}^n$, $y_i \in \mathbb{R}$, and a tolerance $\varepsilon > 0$, in ε-SV regression we aim at finding a function f such that

$$|f(x_i) - y_i| \leq \varepsilon, \ \ i = 1, .., \ell$$

and it fulfills suitable properties (for example, it is as flat as possible)



In a linear regression, we consider an affine function $f(x) = w^{\mathsf{T}}x + b$ and set a tolerance parameter $\varepsilon > 0$.

If we want f to be flat, then we must seek for a small w, which leads us to solve the convex quadratic optimization problem

$$\begin{cases} \min\limits_{w,b} \ \dfrac{1}{2}\|w\|^2 \\ y_i \leq w^{\mathsf{T}}x_i + b + \varepsilon \qquad \forall\ i = 1, \dots, \ell \\ y_i \geq w^{\mathsf{T}}x_i + b - \varepsilon \qquad \forall\ i = 1, \dots, \ell \end{cases} \tag{4}$$

In matrix form (4) becomes:

$$\begin{cases} \min\limits_{w,b} \ \frac{1}{2}(w^T, b)Q\begin{pmatrix} w \\ b \end{pmatrix} \\ D\begin{pmatrix} w \\ b \end{pmatrix} \leq d \end{cases}$$

where

$$Q = \begin{pmatrix} I_n & 0_n \\ 0_n^T & 0 \end{pmatrix} \quad D = \begin{pmatrix} -X & -e_\ell \\ X & e_\ell \end{pmatrix} \quad d = \begin{pmatrix} \varepsilon e_\ell - y \\ \varepsilon e_\ell + y \end{pmatrix}$$

and X is a $\ell \times n$ matrix with row i given by x_i^T, $i = 1, .., \ell$.

Remark

If $x_i \in \mathbb{R}$, then $X = x := (x_1, x_2, ..., x_\ell)^T$ so that

$$D = \begin{pmatrix} -x & -e_\ell \\ x & e_\ell \end{pmatrix}$$

Exercise 6.2. Apply the linear ε-SV regression model with $\varepsilon = 0.5$ to the following training data

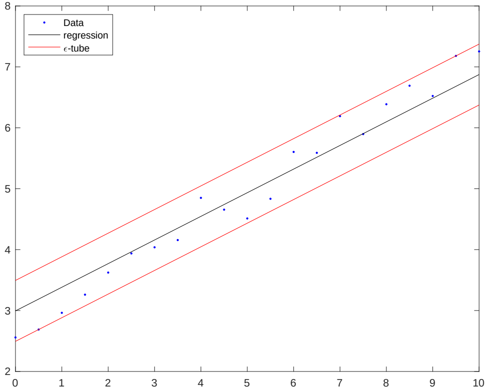
$$\begin{pmatrix} 0 & 2.5584 \\ 0.5000 & 2.6882 \\ 1.0000 & 2.9627 \\ 1.5000 & 3.2608 \\ 2.0000 & 3.6235 \\ 2.5000 & 3.9376 \\ 3.0000 & 4.0383 \\ 3.5000 & 4.1570 \\ 4.0000 & 4.8498 \\ 4.5000 & 4.6561 \\ 5.0000 & 4.5119 \\ 5.5000 & 4.8346 \\ 6.0000 & 5.6039 \\ 6.5000 & 5.5890 \\ 7.0000 & 6.1914 \\ 7.5000 & 5.8966 \\ 8.0000 & 6.3866 \\ 8.5000 & 6.6909 \\ 9.0000 & 6.5224 \\ 9.5000 & 7.1803 \\ 10.0000 & 7.2537 \end{pmatrix}$$

Matlab commands

```
data=[ ]
x = data(:,1) ;
y = data(:,2) ;
l = length(x) ; % number of points
epsilon = 0.5 ;

Q = [ 1 0; 0 0 ];
c = [0;0];
D = [-x -ones(l,1); x ones(l,1)];
d = epsilon*ones(2*l,1) + [-y;y];

sol = quadprog(Q,c,D,d);
w = sol(1);
b = sol(2);
z = w.*x + b ;
zp = w.*x + b + epsilon ;
zm = w.*x + b - epsilon ;

% plot the solution

plot(x,y,'b.',x,z,'k-',x,zp,'r-',x,zm,'r-');
legend('Data','regression','ϵ-tube',... 'Location','NorthWest')
```

w =
0.3880

b =
2.9942



If ε is too small, the model (4) might not be feasible.

The linear ε-SV regression model can be extended by introducing slack variables ξ^+ and ξ^- to relax the constraints of problem (4):

$$\begin{cases} \min\limits_{w,b,\xi^+,\xi^-} \ \dfrac{1}{2}\|w\|^2 + C\displaystyle\sum_{i=1}^{\ell}(\xi_i^+ + \xi_i^-) \\ y_i \le w^{\mathsf{T}}x_i + b + \varepsilon + \xi_i^+ \qquad \forall\ i = 1,\dots,\ell \\ y_i \ge w^{\mathsf{T}}x_i + b - \varepsilon - \xi_i^- \qquad \forall\ i = 1,\dots,\ell \\ \xi^+ \ge 0 \\ \xi^- \ge 0 \end{cases} \tag{5}$$

where parameter C gives the trade-off between the flatness of f and tolerance to deviations larger than ε.

In matrix form (5) becomes:

$$\begin{cases} \min\limits_{w,b} \ \frac{1}{2}(w^T, b, (\xi^+)^\mathsf{T}, (\xi^-)^\mathsf{T}) Q1 \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} + c^\mathsf{T} \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} \\ D1 \begin{pmatrix} w \\ b \\ \xi^+ \\ \xi^- \end{pmatrix} \leq d1 \\ \xi^+ \geq 0, \ \xi^- \geq 0 \end{cases}$$

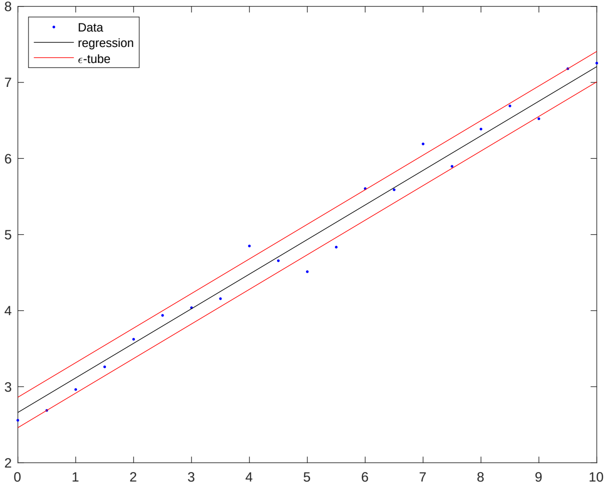
where

$$Q1 = \begin{pmatrix} I_n & 0_n & O_{n\times 2\ell} \\ 0_n^T & 0 & 0_{2\ell}^T \\ O_{2\ell\times n} & 0_{2\ell} & O_{2\ell\times 2\ell} \end{pmatrix} \quad c^T = (O_n^T, 0, C * e_\ell^T, C * e_\ell^T)$$

$$D1 = \begin{pmatrix} -X & -e_\ell & -I_\ell & O_{\ell\times\ell} \\ X & e_\ell & O_{\ell\times\ell} & -I_\ell \end{pmatrix} \quad d = \begin{pmatrix} \varepsilon e_\ell - y \\ \varepsilon e_\ell + y \end{pmatrix}$$

and X is a $\ell \times n$ matrix with row i given by x_i^T, $i = 1, .., \ell$.

Exercise 6.3. Apply the linear ε-SV regression model with slack variables (set $\varepsilon = 0.2$ and $C = 10$) to the training data given in Exercise 6.2.



Linear ε-SV regression with slack variables - dual problem

Let us compute the dual of problem (5). The Lagrangian function is

$$L(\underbrace{w, b, \xi^+, \xi^-}_{\text{primal var.}}, \underbrace{\lambda^+, \lambda^-, \eta^+, \eta^-}_{\text{dual var.}}) = \frac{1}{2}\|w\|^2 - w^\mathsf{T}\left[\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i\right] - b\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)$$

$$+\sum_{i=1}^{\ell}\xi_i^+(C - \lambda_i^+ - \eta_i^+) + \sum_{i=1}^{\ell}\xi_i^-(C - \lambda_i^- - \eta_i^-) - \varepsilon\sum_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum_{i=1}^{\ell}y_i(\lambda_i^+ - \lambda_i^-)$$

If $\sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) \neq 0$ or $C - \lambda_i^+ - \eta_i^+ \neq 0$ for some i or $C - \lambda_i^- - \eta_i^- \neq 0$ for some i, then $\min_{w,b,\xi^+,\xi^-} L = -\infty$. Otherwise,

$$\nabla_w L = w - \sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i = 0.$$

Operating as in previously made calculations, we substitute $w = \sum_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-)x_i$ in the Lagrangian and we consider the above mentioned constraints.

The dual problem of (5) is

$$
\begin{cases}
\max\limits_{\lambda^+,\lambda^-,\eta^+,\eta^-\geq 0} \; -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+-\lambda_i^-)(\lambda_j^+-\lambda_j^-)(x_i)^{\mathsf{T}}x_j \\
\qquad\qquad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+-\lambda_i^-) \\
\sum\limits_{i=1}^{\ell}(\lambda_i^+-\lambda_i^-) = 0 \\
C-\lambda_i^+-\eta_i^+ = 0, \;\; i=1,..,\ell \\
C-\lambda_i^--\eta_i^- = 0, \;\; i=1,..,\ell
\end{cases}
$$

Finally, eliminating the variables η_i^+, η_i^- we obtain:

$$
\begin{cases}
\max\limits_{\lambda^+,\lambda^-} \; -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+-\lambda_i^-)(\lambda_j^+-\lambda_j^-)(x_i)^{\mathsf{T}}x_j \\
\qquad\qquad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+-\lambda_i^-) \\
\sum\limits_{i=1}^{\ell}(\lambda_i^+-\lambda_i^-) = 0 \\
\lambda_i^+ \in [0, C], \;\; i=1,..,\ell \\
\lambda_i^- \in [0, C], \;\; i=1,..,\ell
\end{cases}
$$

Let us write the dual problem in matrix form.

Consider first the quadratic part of the objective function.

It is possible to show that, setting

$$X = [(x_i)^\mathsf{T} x_j] \quad i,j = 1,..,\ell, \qquad Q = \begin{pmatrix} X & -X \\ -X & X \end{pmatrix}, \tag{6}$$

then, we have:

$$-\frac{1}{2}\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j = -\frac{1}{2}((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T}) Q \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix}$$

Indeed, note that

$$\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)(x_i)^\mathsf{T} x_j$$

$$= \sum_{i=1}^{\ell}\sum_{j=1}^{\ell}(\lambda_i^+\lambda_j^+ - \lambda_i^+\lambda_j^- - \lambda_i^-\lambda_j^+ + \lambda_i^-\lambda_j^-)(x_i)^\mathsf{T} x_j \tag{7}$$

Moreover,

$$((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T}) Q \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix} = ((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T}) \begin{pmatrix} X & -X \\ -X & X \end{pmatrix} \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix} =$$

$$= [(\lambda^+)^\mathsf{T} X - (\lambda^-)^\mathsf{T} X]\lambda^+ + [(\lambda^+)^\mathsf{T}(-X) + (\lambda^-)^\mathsf{T} X]\lambda^-$$

$$= (\lambda^+)^\mathsf{T} X \lambda^+ - (\lambda^-)^\mathsf{T} X \lambda^+ - (\lambda^+)^\mathsf{T} X \lambda^- + (\lambda^-)^\mathsf{T} X \lambda^-$$

which equals (7).

Finally, we obtain:

Dual problem in matrix form

$$\begin{cases} \max\limits_{\lambda^+, \lambda^-} \; -\dfrac{1}{2}((\lambda^+)^\mathsf{T}, (\lambda^-)^\mathsf{T}) Q \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix} + [-\epsilon(e_\ell^\mathsf{T}, e_\ell^\mathsf{T}) + (y^\mathsf{T}, -y^\mathsf{T})] \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix} \\ (e_\ell^\mathsf{T}, -e_\ell^\mathsf{T}) \begin{pmatrix} \lambda^+ \\ \lambda^- \end{pmatrix} = 0 \\ \lambda_i^+ \in [0, C], \;\; i = 1, .., \ell \\ \lambda_i^- \in [0, C], \;\; i = 1, .., \ell \end{cases}$$

where Q is defined by (6).

- Dual problem is a convex quadratic programming problem
- If $\lambda_i^+ > 0$ or $\lambda_i^- > 0$, then x_i is said support vector
- If (λ^+, λ^-) is a dual optimum, then

$$w = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-) x_i, \tag{8}$$

- b is obtained using the complementarity conditions:

$$\begin{array}{l} \lambda_i^+ \left[\varepsilon + \xi_i^+ - y_i + w^\mathsf{T} x_i + b \right] = 0 \\ \lambda_i^- \left[\varepsilon + \xi_i^- + y_i - w^\mathsf{T} x_i - b \right] = 0 \\ \xi_i^+ (C - \lambda_i^+) = 0 \\ \xi_i^- (C - \lambda_i^-) = 0 \end{array}$$

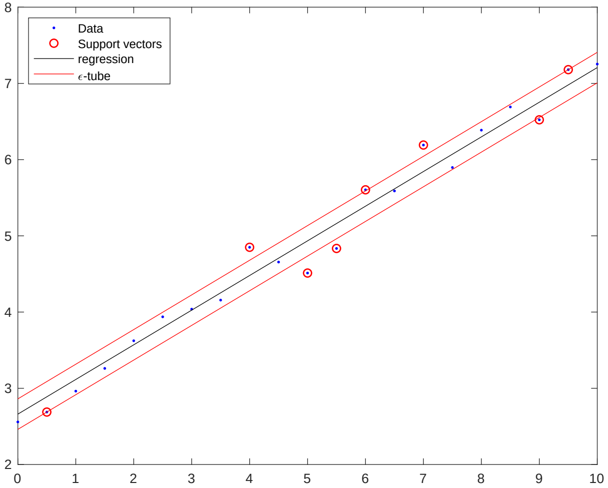
Hence, if there is some i s.t. $0 < \lambda_i^+ < C$, then

$$b = y_i - w^\mathsf{T} x_i - \varepsilon; \tag{9}$$

while, if there is some i s.t. $0 < \lambda_i^- < C$, then

$$b = y_i - w^\mathsf{T} x_i + \varepsilon. \tag{10}$$

Exercise 6.4. Solve the dual problem of the linear ε-SV regression model with slack variables (set $\varepsilon = 0.2$ and $C = 10$) applied to the training data given in Exercise 6.2.



Matlab commands

```
data=[ .....]

x = data(:,1) ; y = data(:,2) ; l = length(x) ; epsilon = 0.2 ; C = 10;

X = zeros(l,l);
for i = 1 : l
    for j = 1 : l
        X(i,j) = x(i)*x(j);
    end
end
Q = [ X -X ; -X X ];
c = epsilon*ones(2*l,1) + [-y;y];

% solve the problem

sol = quadprog(Q,c,[],[],[ones(1,l) -ones(1,l)],0,zeros(2*l,1),C*ones(2*l,1));
lap = sol(1:l);
lam = sol(l+1:2*l);

% compute w

w = (lap-lam)'*x ;
```

Matlab commands (continued)

```
% compute b

ind = find(lap > 0.001 & lap < C- 0.001);
if isempty(ind)==0
i = ind(1);
b = y(i) - w*x(i) - epsilon ;
else
ind = find(lam > 0.001 & lam < C- 0.001);
i = ind(1);
b = y(i) - w*x(i) + epsilon ;
end

% find regression and epsilon-tube

z = w.*x + b ;
zp = w.*x + b + epsilon ;
zm = w.*x + b - epsilon ;

% find support vectors and plot the solution

sv = [find(lap > 1e-3);find(lam > 1e-3)];
sv = sort(sv);

plot(x,y,'b.',x(sv),y(sv), 'ro',x,z,'k-',x,zp,'r-',x,zm,'r-');
```

Nonlinear ε-SV regression

In order to generate a nonlinear regression function f, we can use the kernel functions (see part 5 related to classification problems).

Consider a map $\phi : \mathbb{R}^n \to \mathcal{H}$ (associated to a kernel function), where $\mathcal{H}$ (features space) is a higher dimensional (maybe infinite) space and find a linear regression for the points $\{(\phi(x_i), y_i)\}$ in the space $\mathcal{H} \times \mathbb{R}$.

The primal problem becomes:

$$\begin{cases} \min \ \dfrac{1}{2}\|w\|^2 + C \displaystyle\sum_{i=1}^{\ell} (\xi_i^+ + \xi_i^-) \\ y_i \leq w^{\mathsf{T}} \phi(x_i) + b + \varepsilon + \xi_i^+ \qquad \forall\ i = 1, \dots, \ell \\ y_i \geq w^{\mathsf{T}} \phi(x_i) + b - \varepsilon - \xi_i^- \qquad \forall\ i = 1, \dots, \ell \end{cases}$$

where w is a vector in a high (possibly infinite) dimensional space called the dual space of $\mathcal{H}$.

The dual problem is:

$$\begin{cases} \max\limits_{(\lambda^+,\lambda^-)} & -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)\phi(x_i)^\mathsf{T}\phi(x_j) \\ & \quad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\ \sum\limits_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 \\ \lambda_i^+, \lambda_i^- \in [0, C] \end{cases}$$

or,

$$\begin{cases} \max\limits_{(\lambda^+,\lambda^-)} & -\dfrac{1}{2}\sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{\ell}(\lambda_i^+ - \lambda_i^-)(\lambda_j^+ - \lambda_j^-)k(x_i, x_j) \\ & \quad -\varepsilon\sum\limits_{i=1}^{\ell}(\lambda_i^+ + \lambda_i^-) + \sum\limits_{i=1}^{\ell} y_i(\lambda_i^+ - \lambda_i^-) \\ \sum\limits_{i=1}^{\ell}(\lambda_i^+ - \lambda_i^-) = 0 \\ \lambda_i^+, \lambda_i^- \in [0, C] \end{cases}$$

a finite dimensional problem with 2ℓ variables

- choose a kernel function $k(x, y)$
- solve the dual and find (λ^+, λ^-)
- Recall that, by (8) now we have:

$$w = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)\phi(x_i), \tag{11}$$

and, consequently,

$$w^T\phi(x) = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)\phi(x_i)\phi(x) = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-)k(x_i, x).$$

By (9) and (10) we compute b:

$$b = y_i - \varepsilon - \sum_{j=1}^{\ell} (\lambda_j^+ - \lambda_j^-)k(x_i, x_j), \qquad \text{for some } i \text{ s.t. } 0 < \lambda_i^+ < C$$

or

$$b = y_i + \varepsilon - \sum_{j=1}^{\ell} (\lambda_j^+ - \lambda_j^-)k(x_i, x_j), \qquad \text{for some } i \text{ s.t. } 0 < \lambda_i^- < C$$

(Recall that $k(x_i, x_j) = k(x_j, x_i)$.)

Finally, the regression function is:

$$f(x) = w^\top \phi(x) + b = \sum_{i=1}^{\ell} (\lambda_i^+ - \lambda_i^-) k(x_i, x) + b$$

Remark

The regression function is

- linear in the features space
- nonlinear in the input space

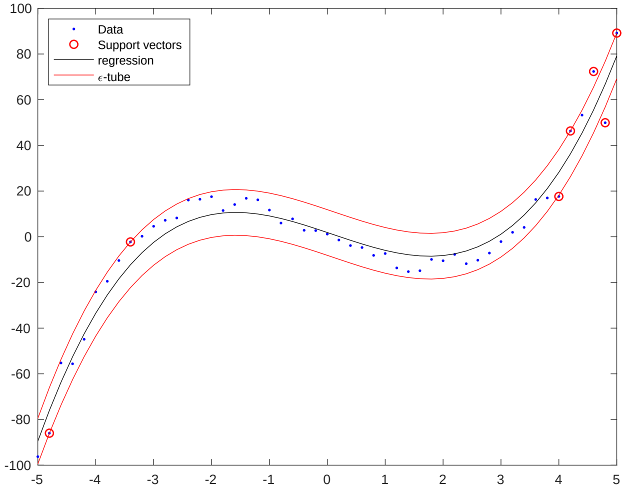
Exercise 6.5. Consider the training data given in Exercise 6.1. Apply the nonlinear ε-SV regression using a polynomial kernel with degree $p = 4$ and parameters $\varepsilon = 10$, $C = 10$. Moreover, find the support vectors.

Matlab commands

```
data=[ .....]

x = data(:,1) ; y = data(:,2) ; l = length(x) ; epsilon = 10 ; C = 10;

X = zeros(l,l); for i = 1 : l
    for j = 1 : l
        X(i,j) = kernel(x(i),x(j));
    end
end
Q = [ X -X ; -X X ];
c = epsilon*ones(2*l,1) + [-y;y];

% solve the problem

sol = quadprog(Q,c,[],[],[ones(1,l) -ones(1,l)],0,zeros(2*l,1),C*ones(2*l,1));
lap = sol(1:l);
lam = sol(l+1:2*l);

% compute b

ind = find(lap > 1e-3 & lap < C-1e-3);
if isempty(ind)==0
i = ind(1);
```

```
b = y(i) - epsilon;
for j = 1 : l
b = b - (lap(j)-lam(j))*kernel(x(i),x(j));
end
else
ind = find(lam > 1e-3 & lam < C-1e-3);
i = ind(1);
b = y(i) + epsilon ;
for j = 1 : l
b = b - (lap(j)-lam(j))*kernel(x(i),x(j));
end
end

% find regression and epsilon-tube evaluating f(x) at x(i), i=1,..,l

z = zeros(l,1);
for i = 1 : l
z(i) = b ;
for j = 1 : l
z(i) = z(i) + (lap(j)-lam(j))*kernel(x(i),x(j));
end
end
zp = z + epsilon ;
zm = z - epsilon ;
```

```
% find support vectors and plot the solution

sv = [find(lap > 1e-3);find(lam > 1e-3)];
sv = sort(sv);
plot(x,y,'b.',x(sv),y(sv), 'ro',x,z,'k-',x,zp,'r-',x,zm,'r-');

% kernel function

function v = kernel(x,y)

p = 4 ;

v = (x'*y + 1)^ p;

end
```


Data
Support vectors
regression
ϵ-tube
100
80
60
40
20
0
-20
-40
-60
-80
-100
-5
-4
-3
-2
-1
0
1
2
3
4
5