OLS with ℓ_1 and ℓ_2 regularization

CEE 629. System Identification

Duke University, Fall 2017

ℓ_1 regularization

- The ℓ_1 norm of a vector $v \in \mathbb{R}^n$ is given by $||v||_1 = \sum |v_i|$
  The gradient of $||v||_1$ is not defined if an element of v is zero.
- In ℓ_1 regularization, the objective $J(a) = ||y - f(y;a)||_2^2$ is penalized with a term $\alpha||a||_1$, where α is called the *regularization parameter*, or the *penalty factor*.
- The effect of ℓ_1 regularization is to force some of the model parameters, a_i, to zero (exactly). If the parameters are coefficients for bases of the model, then ℓ_1 regularization is a means to remove un-important bases of the model. It is a form of model reduction
- It is applicable to linear and nonlinear models.
- It has similar but not identical effects as ℓ_2 regularization and truncated SVD solutions
- a.k.a. LASSO, Compressed Sensing, Support Vector Machine

But ℓ_1 is not smooth at the optimum point.
What can one say about necessary conditions for optimality?

ℓ_1 regularization can be recast as a Quadratic Program (QP)

$$
\begin{aligned}
J(a) &= ||y - Xa||_2^2 + \alpha||a||_1 = ||y - Xa||_2^2 + \alpha \sum_i |a_i| && (1) \\
&\Leftrightarrow \\
& a_i \equiv p_i - q_i && (2) \\
& |a_i| \equiv p_i + q_i && (3) \\
J(p,q) &= ||y - Xp + Xq||_2^2 + \alpha \sum_i (p_i + q_i) && (4) \\
& \quad \text{such that } p_i \geq 0 \text{ and } q_i \geq 0 \quad \forall\ i
\end{aligned}
$$

Five conditions to show that ℓ_1 is a QP

1. $p_i - q_i = a_i$
2. $p_i + q_i = |a_i|$
3. $p_i \geq 0 \quad q_i \geq 0$
4. $a_i > 0 \Rightarrow \; p_i = a_i \;, \quad q_i = 0$
   $a_i < 0 \Rightarrow \; p_i = 0 \;, \quad q_i = -a_i$
   $a_i = 0 \Rightarrow \; p_i = 0 \;, \quad q_i = 0$
5. $\min(p_i + q_i) = a_i$

- (1)&(2) $\Rightarrow$ (3)&(4)
- (1)&(3) $\not\Rightarrow$ (2)&(4)
- (1)&(3) $\Rightarrow$ (4)&(5)

Solving the ℓ_1 regularization QP

$$J(p,q) \;=\; ||y - Xp + Xq||_2^2 + \alpha \sum_i (p_i + q_i)$$
$$\text{such that } p_i \geq 0 \text{ and } q_i \geq 0 \quad \forall \; i$$

But which elements of p_i and which elements of q_i should be set to zero?
... (the "active" constraints)
This question does not have an answer in closed form.
So we solve the problem incrementally.

Incremental formulation

$$p^{(k+1)} \;=\; p^{(k)} + u^{(k)} \quad , \quad p^{(k)} + u^{(k)} \geq 0 \tag{5}$$
$$q^{(k+1)} \;=\; q^{(k)} + v^{(k)} \quad , \quad q^{(k)} + v^{(k)} \geq 0 \tag{6}$$

Lagrangian

$$L(p,q,\mu,\nu) = J(p,q) + \mu_{i\in A_u}^{(k)\mathsf{T}}(p^{(k)} + u^{(k)})_{i\in A_u} + \nu_{i\in A_v}^{(k)\mathsf{T}}(q^{(k)} + v^{(k)})_{i\in A_v}$$

- k is the iteration number
- A_u is the set of active equality constraints $p_i = 0$
- A_v is the set of active equality constraints $q_i = 0$
- $\mu_{i\in A_u}^{(k)}$ is the set of Lagrange multipliers for the active constraint set A_u
- $\nu_{i\in A_v}^{(k)}$ is the set of Lagrange multipliers for the active constraint set A_v

Minimize the Lagrangian w.r.t. (p, q),

Maximize the Lagrangian w.r.t. (μ, ν)

$$
\begin{aligned}
L = y^\mathsf{T} y \ & -2(p+u)^\mathsf{T} X^\mathsf{T} y + p^\mathsf{T} \alpha \\
& +2(q+v)^\mathsf{T} X^\mathsf{T} y + q^\mathsf{T} \alpha \\
& +(p+u)^\mathsf{T} X^\mathsf{T} X (p+u) \\
& -2(q+v)^\mathsf{T} X^\mathsf{T} X (p+u) \\
& +\mu_{i \in A_u}^\mathsf{T} (p+u)_{i \in A_u} \\
& +\nu_{i \in A_v}^\mathsf{T} (q+v)_{i \in A_v}
\end{aligned}
$$

The necessary conditions for optimality ...

$$\frac{\partial L}{\partial u} = 0 : -2X^\mathsf{T} y + \alpha + \mu_{i \in A_u} + 2X^\mathsf{T} X p + 2X^\mathsf{T} X u - 2X^\mathsf{T} X q - 2X^\mathsf{T} X v = 0$$

$$\frac{\partial L}{\partial v} = 0 : +2X^\mathsf{T} y + \alpha + \nu_{i \in A_v} - 2X^\mathsf{T} X p - 2X^\mathsf{T} X u + 2X^\mathsf{T} X q + 2X^\mathsf{T} X v = 0$$

$$\frac{\partial L}{\partial \mu_{i \in A_u}} = 0 : (p+u)_{i \in A_u} = 0$$

$$\frac{\partial L}{\partial \nu_{i \in A_v}} = 0 : (q+v)_{i \in A_v} = 0$$

... are linear in our unknowns u, v, μ, ν ...

$$
\begin{bmatrix}
2X^\mathsf{T} X & -2X^\mathsf{T} X & I_{i \in A_u}^\mathsf{T} & \\
-2X^\mathsf{T} X & 2X^\mathsf{T} X & & I_{i \in A_v}^\mathsf{T} \\
I_{i \in A_u} & & & \\
& I_{i \in A_v} & &
\end{bmatrix}
\begin{bmatrix} u \\ v \\ \mu \\ \nu \end{bmatrix}
=
\begin{bmatrix}
2X^\mathsf{T} y - 2X^\mathsf{T} X p + 2X^\mathsf{T} X q - \alpha \\
-2X^\mathsf{T} y + 2X^\mathsf{T} X p - 2X^\mathsf{T} X q - \alpha \\
-p_{i \in A_u} \\
-q_{i \in A_v}
\end{bmatrix}
$$

The number of columns of the matrix $I_{i \in A_u}$ is the number of model parameters. The number of rows of $I_{i \in A_u}$ is the number of active constraints on p. If index i is the element j in the set of active constraints, A_u, then the i, j element of $I_{i \in A_u}$ equals 1.

A trick to block an incremental step from going negative.

Define the index j s.t. $p_j + u_j = \min(p + u)$ ... $(p_j \geq 0)$

If $p_j + u_j < 0$, then define $\delta_u = -p_j/u_j$ $(\delta_u > 0)$
and adjust the increment by the factor δ_u

$$p^{(k+1)} = p^{(k)} + \delta_u u^{(k)}$$

Likewise ...

Define the index j s.t. $q_j + v_j = \min(q + v)$ ... $(q_j \geq 0)$

If $q_j + v_j < 0$, then define $\delta_v = -q_j/v_j$ $(\delta_v > 0)$
and adjust the increment by the factor δ_v

$$q^{(k+1)} = q^{(k)} + \delta_v v^{(k)}$$

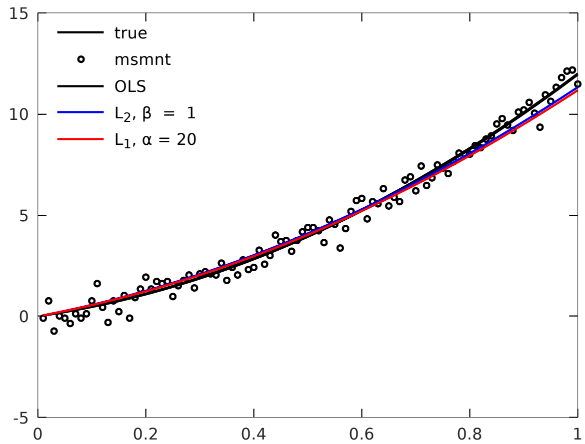
Implementation in L1_fit.m

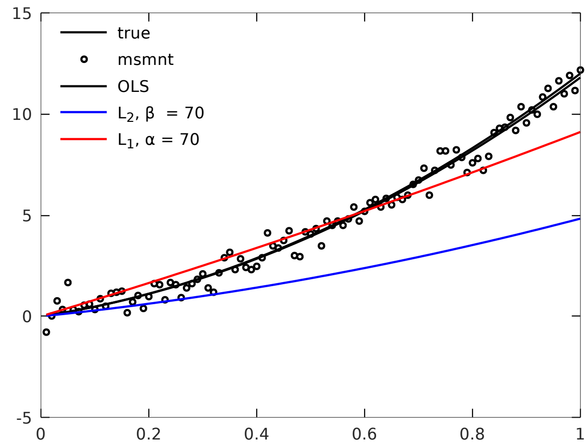
Example 1, 2-term power polynomial

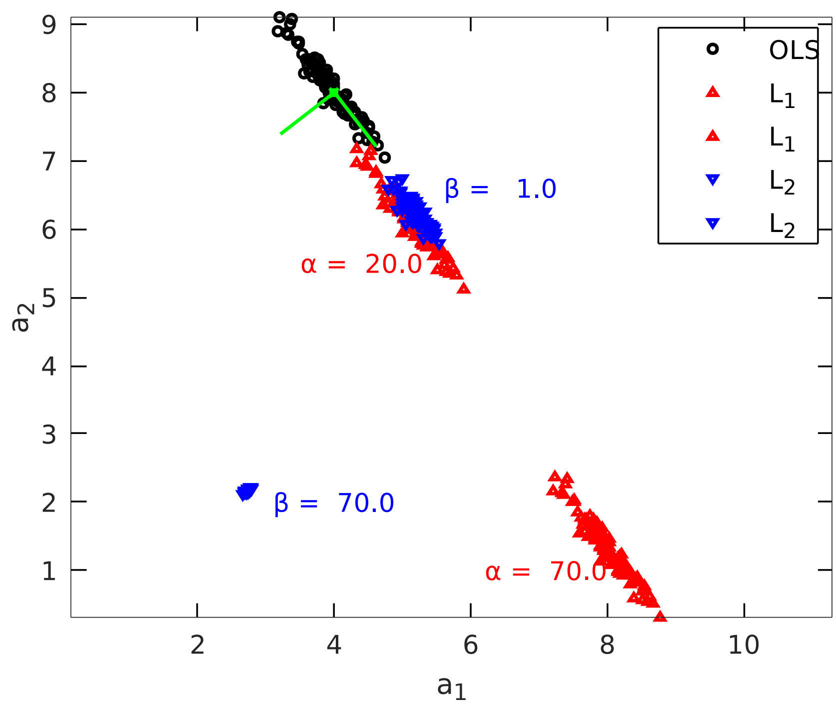
$$\hat{y}(x; a_1, a_2) = a_1 x + a_2 x^2 \qquad y = \hat{y} + \eta \qquad \sigma_\eta = 0.5$$

$$(a_1 = 4, a_2 = 8)$$

OLS criterion	$\min_a \|\|y - Xa\|\|_2^2$
ℓ_1 regularization criterion	$\min_a \|\|y - Xa\|\|_2^2 + \alpha\|\|a\|\|_1$
ℓ_2 regularization criterion	$\min_a \|\|y - Xa\|\|_2^2 + \beta\|\|a\|\|_2$







Example 2, 100-term Prony Series

A Prony series a model for the behavior dynamic system expressed in terms of a convolution of the system forcing with a kernel, in which the kernel is a series of exponentials.

$$y(t) = \int_0^t h(r) u(t-r) \; dr$$

where, for example, the kernel can be parameterized as

$$h(r) = k_0 + \sum_{i=1}^{n} k_i \exp[-r/\tau_i]$$

Prony series are linear in the coefficients k_i but are highly nonlinear in the time constants τ_i.

In the frequency domain, the complex modulus is obtained from the Fourier transform of the convolution kernel,

$$\hat{H}(\omega) = k_0 + \sum_{i=1}^{n} k_i \, \frac{\mathrm{i}\omega\tau_i}{1 + \mathrm{i}\omega\tau_i}$$

The real part of $\hat{H}(\omega)$ is called the *storage modulus* and represents the energy-conserving elasticity of the system. The imaginary part of $\hat{H}(\omega)$ is called the *loss modulus* and relates to the energy dissipation aspects. For linear visco-elastic materials the loss modulus approaches zero as ω approaches zero.

Using ℓ_1 regularization, a Prony series with very large set of time constants can be fit to complex-modulus data. By tuning the ℓ_1 penalty factor α to be large enough, a large number of coefficients in the Prony series will be forced to zero. Since negative values of the coefficients are not permissible, this problem is a perfect candidate for ℓ_1 regularization.

The system model is then given by

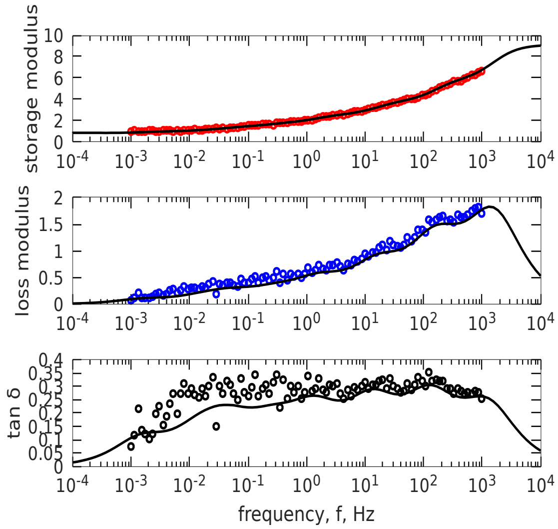
$$\hat{H}(\omega; k) = T(\tau) k$$

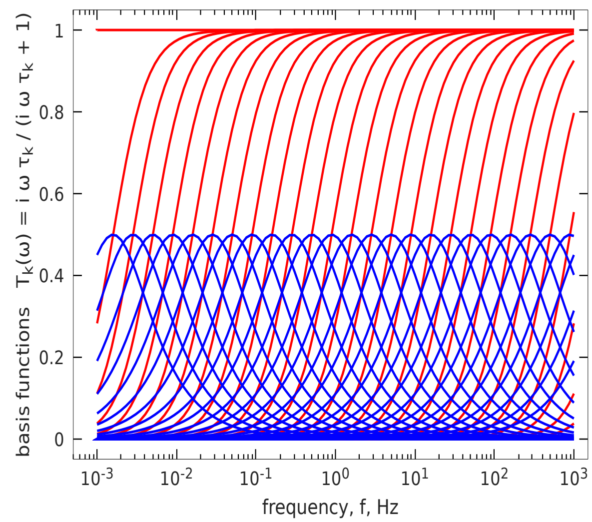
where the i-th column of the matrix $T(\tau)$ is $\mathrm{i}\omega\tau_i/(1 + \mathrm{i}\omega\tau_i)$ and the vector k contains the $n + 1$ coefficients $k_0, ..., k_n$.

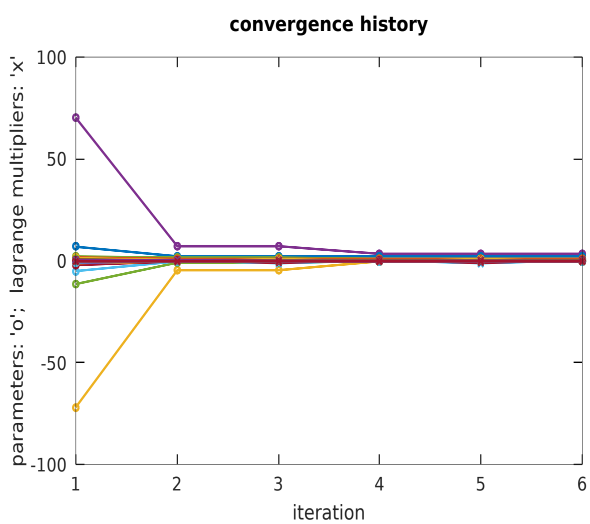
The regularized objective function is

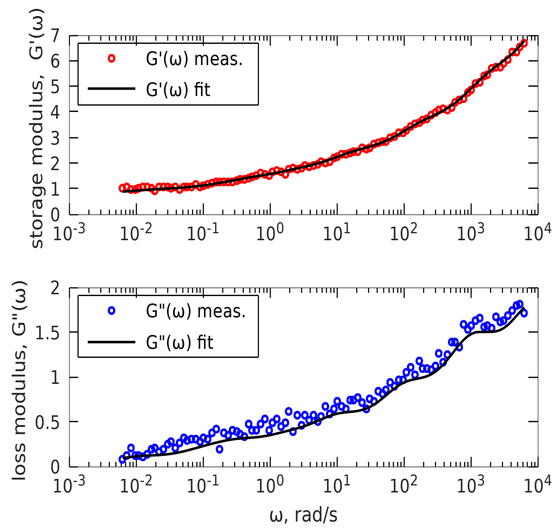
$$J(k) = ||H(\omega) - T(\tau)k||_2^2 + \alpha \sum_i k \quad \text{s.t. } k \geq 0$$

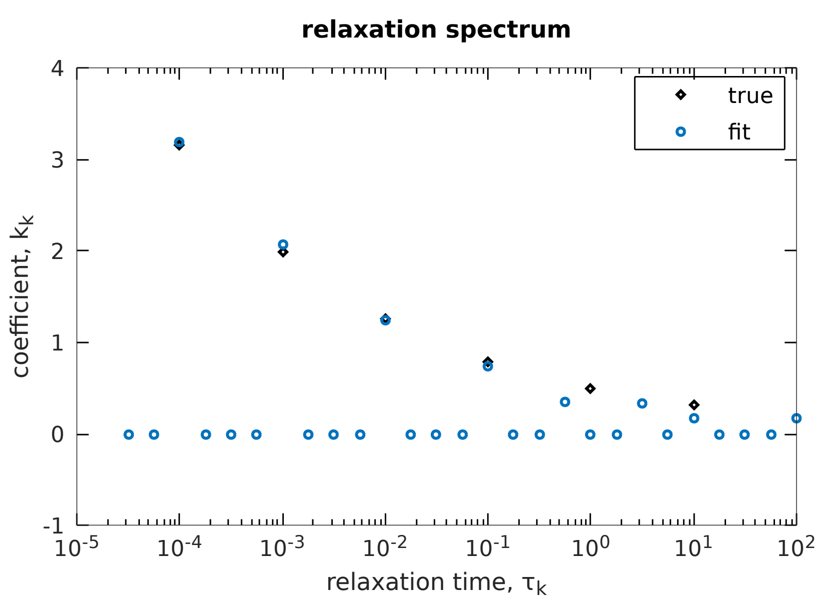
This is a special (more simple) case of the ℓ_1 objective analyzed in the previous section. The solution is implemented in PronyFit.m .


storage modulus
loss modulus
tan δ
frequency, f, Hz


basis functions $T_k(\omega) = i\,\omega\,\tau_k / (i\,\omega\,\tau_k + 1)$
frequency, f, Hz


convergence history
parameters: 'o'; lagrange multipliers: 'x'
iteration


G'(ω) meas.
G'(ω) fit
storage modulus, G'(ω)
G"(ω) meas.
G"(ω) fit
loss modulus, G"(ω)
ω, rad/s


relaxation spectrum
true
fit
coefficient, k_k
relaxation time, τ_k

L1_reg_example.m

```
% L1_reg_example.m
% HPG, Duke Univ. 2013-09, 2017-09

% generate some data (x,y), noisy in y

m = 100;                        % number of measurement points
x = [ 1:m]'/m;                  % independent variables - noise-free

a = [ 4 8 ]';                   % "true" parameter coefficients
n = length(a);

X = zeros(m,n);
for i=1:n
        X(:,i) = x.^i;
end

[eigvec,eigval] = eig(X'*X);    % principal directions of parameter covariance

y = X*a;

alpha_set = [ 20.0  70.0 ];     % for L1 regularization
beta_set  = [  1.0  70.0 ];     % for L2 regularization

N_MCS = 100;
N_R   = length(alpha_set);

a_hat_ols_rec   = zeros(n,N_MCS);
a_hat_alpha_rec = zeros(n,N_R,N_MCS);
a_hat_beta_rec  = zeros(n,N_R,N_MCS);


for j=1:N_MCS;                  % ... start simulation loop

 y_dat = y + 0.5*randn(m,1);            % add noise to true data

 a_hat_ols = X \ y_dat;                                 % ordinary least squares
 y_hat_ols = X*a_hat_ols;

 a_hat_ols_rec(:,j) = a_hat_ols;

 for k=1:N_R

  alpha = alpha_set(k);
  beta  = beta_set(k);

  a_hat_alpha = L1_fit ( X, y_dat, alpha );             % L_1 regularization
  y_hat_alpha = X * a_hat_alpha;
  a_hat_alpha_rec(:,j,k) = a_hat_alpha;

  a_hat_beta = [ X'*X + beta*eye(n) ] \ X'*y_dat;       % L_2 regularization
  y_hat_beta = X*a_hat_beta;
  a_hat_beta_rec(:,j,k)  = a_hat_beta;

  figure(1)
   clf
    plot( x,y,'-k', x,y_dat,'ok', ...
          x,y_hat_ols,'-k', x,y_hat_beta,'-b', x,y_hat_alpha,'-r' )
    legend('true','msmnt','OLS', ...
        sprintf('L_2, \\beta  = %2.0f',beta),  ...
        sprintf('L_1, \\alpha = %2.0f',alpha),'location','northwest');
    legend('boxoff')
   drawnow

 end

end                             % ... end simulation loop
```

L1_fit.m

```
function [a, mu, nu, cvg_hst] = L1_fit ( X, y, alpha )
% [a, mu, nu, cvg_hst] = L1_fit(X,y,alpha)
%
% fit model parameters, a, in the model ^y = X*a  to data, y, with
% L1 regularizaion of the parameters.
%   J  = ||  y - X*a  ||_2^2    +   alpha * ||a||_1
%  <=>
%   J = ||  y - X(p-q) ||_2^2  +   alpha * sum(p+q)  such that  p>=0, q>=0
%   (a = p-q; |a| = p+q)
%
% INPUT:  X     ...  the design matrix (basis of the model),      m x n
%         y     ...  the vector of data to be fit to the model,   m x 1
%        alpha  ...  l_1 regularization factor for Prony series coefficients
%
% OUTPUT: a         ...  the model coefficients
%         mu,nu      ... Lagrange multipliers for p and q
%         cvg_hst  ...  convergence history
%

%{
   The main idea behind casting L1 as a QP is that the parameter
vector {a} is replaced by the difference of two vectors {a}={p}-{q}
that are constrained to be non-negative: p_i >=0 for all i and q_i >=0
for all i.
  If a_i > 0, then p_i=a_i and q_i=0;
  If a_i < 0, then p_i= 0  and q_i = -a_i.
 With this constrained re-parameterization, |a_i| = p_i + q_i.
 Note that the dimension of the parameter space doubles, but the KTT equations
 for the QP are simple and have analytical Hessians and gradients.
%}


 [m,n] = size(X);

 t = [1:m];

 XtX = 2*X'*X;  Xty = 2*X'*y;

% _good_ initial guess for p and q from non-regularized linear least squares
 a  = XtX \ Xty;
 p  = zeros(n,1);       p (find(a >  2*eps)) =  a(find(a >  2*eps));
 q  = zeros(n,1);       q (find(a < -2*eps)) = -a(find(a < -2*eps));

 MaxIter = 19;

 cvg_hst = zeros ( 5*n, MaxIter );             % convergence history

 for iter = 1:MaxIter

   Au = find(p <= 2*eps);       lp = length(Au);   % active set for update u
   Av = find(q <= 2*eps);       lq = length(Av);   % active set for update v

   Ip = zeros(lp,n); for i=1:lp, Ip(i,Au(i)) = 1; end   % constraint gradient u
   Iq = zeros(lq,n); for i=1:lq, Iq(i,Av(i)) = 1; end   % constraint gradient v

   mu = zeros(n,1); nu = zeros(n,1);
   % KKT equations
   XTX = [  XtX       -XtX     Ip'        zeros(n,lq)  ;         % dL/du   = 0
           -XtX        XtX   zeros(n,lp)  Iq'          ;         % dL/dv   = 0
              Ip        zeros(lp,n+lp+lq)              ;         % dL/d mu = 0
          zeros(lq,n)   Iq   zeros(lq,lp+lq)          ];         % dL/d nu = 0

   % right-hand-side vector
   XTY = [ Xty - XtX*p + XtX*q - alpha ;                         % dL/du   = 0
          -Xty + XtX*p - XtX*q - alpha ;                         % dL/dv   = 0
           -p(Au)                      ;                         % dL/d mu = 0
           -q(Av)                      ];                        % dL/d nu = 0

   u_v_mu_nu = XTX \ XTY;               % solve the system
```

```
%
```

```
    u      = u_v_mu_nu(1:n);                    % update for p
    v      = u_v_mu_nu(n+1:2*n);                % update for q
    mu(Au) = u_v_mu_nu(2*n+1:2*n+lp);           % what to use mu for?
    nu(Av) = u_v_mu_nu(2*n+lp+1:2*n+lp+lq);     % what to use nu for?

    % if an element of p+u becomes negetive, reduce the length of step u
    du = 1;
    [p_min, j] = min(p+u);
    if p_min < 0
             du = -p(j)/u(j);
    end

    % if an element of q+v becomes negetive, reduce the length of step v
    dv = 1;
    [q_min, j] = min(q+v);
    if q_min < 0
             dv = -q(j)/v(j);
    end

    p = p + du*u;
    q = q + dv*v;
    a = p - q;

    cvg_hst(:,iter) = [ a ; p ; q ; mu ; nu ];   % convergence history

    % convergence check
    if ( norm(u) <= norm(p)/1e3  &&  min(p) > -5*eps  && ...
         norm(v) <= norm(q)/1e3  &&  min(q) > -5*eps )
         break;
    end

%   figure(101); clf; plot(t,y,'o', t,X*a); drawnow;

  end

  cvg_hst = cvg_hst(:,1:iter);

% figure(102); clf; plot([1:iter], cvg_hst(1:n,:)' ,'-o'); drawnow; %pause(1);

% ------------------------------------------------------------------ L1_fit
% H.P. Gavin, 2013-10-04
```

PronyFit_test.m

```
% --- PronyFit_test.m
% test prony series fitting with L1 regularization

clear all

% simulated noisy data

% a relatively small number of 'true' time lags
tau = 1e-2*[ 0.01 0.1 1 10 100 1000 ]';
ko  = 1;                                    % static stiffness
k   = 0.5 ./ tau.^0.2;                      % 'true' Prony series coefficients

points = 100;
f_dat = logspace(-3,3,points)';
iw = 2*pi*f_dat * sqrt(-1.0);

% generate complex modulus data with some additive noise and friction effects
T = [ ones(points,1) ,  iw*tau' ./ (iw*tau' + 1.0) ];
G_dat = T * [ ko ; k ] + 5e-2*(randn(points,1) + i*randn(points,1));

friction = 0.1;                   % definately NOT linear viscoelasticity!
G_dat = real(G_dat) + sqrt(-1)*(friction + imag(G_dat));

% plot the simulated data
figure(1)
 clf
% semilogx(f,real(G),'or',f,imag(G),'ob')
  subplot(311)
   semilogx(f_dat,real(G_dat),'or')
    ylabel('storage modulus')
  subplot(312)
   semilogx(f_dat,imag(G_dat),'ob')
    ylabel('loss modulus')
  subplot(313)
   semilogx(f_dat,imag(G_dat)./real(G_dat),'ok')
    ylabel('tan \delta')
    xlabel('frequency, f_{dat}, Hz')

% number of terms in the Prony series
nID = 97;

tau_id = logspace(-4.5,2,nID)';             % specified set of time lags, tau

alpha = 0.50;                               % l_1 regularization parameter

[ko_id,k_id,cvg_hst] = PronyFit(G_dat,f_dat,tau_id,alpha); % do it!

f_fit  = logspace(-4,4,100);
iw_fit = 2*pi*f_fit * sqrt(-1.0);
G_fit  = ko_id + sum( (k_id.*tau_id * iw_fit) ./ (tau_id * iw_fit + 1) );
```


PronyFit.m

```
function [ko,k,cvg_hst] = PronyFit(G_dat,f_dat,tau,alpha)
% [ko,k,cvg_hst] = prony_fit(G_dat,f_dat,tau,alpha)
%
%  Fit a prony series to frequency domain complex modulus data
%
% INPUT:   G_dat   ...  complex modulus data                         Mx1 complex vector
%          f_dat   ...  frequencies where the measured frequency response data is
%                       evaluated  (Hz),   (f>0)                     Mx1 real vector
%           tau    ...  specified set of relaxation times,           Nx1 real vector
%         alpha    ...  l_1 regularization factor for Prony series coefficients
%
% OUTPUT: ko, k       ...   Prony series coefficients
%          cvg_hst    ...   convergence history


 i = sqrt(-1.0);

 m  = length(f_dat);                                        % number of data points
 w  = 2*pi * f_dat;                                         % one-sided frequency

 T = [ ones(m,1)  ,  i*w*tau' ./ (i*w*tau' + 1.0) ];       % design matrix

% plot the basis functions (columns of T) with single-sided log-scale frequencies
figure(101)
 semilogx(f_dat, real(T), '-r', f_dat, imag(T),'-b')
  ylabel('basis functions   T_k(\omega) = i \omega \tau_k / (i \omega \tau_k + 1)')
  xlabel('frequency, f, Hz')
  axis( [ 0.5*min(f_dat) 1.5*max(f_dat) -0.05 1.05 ]  )

 [m,n] = size(T);       % m = number of data points; n = number of parameters

 TtT = 2*real(T'*T);    % taking real part is like adding complex conjugate
 TtG = 2*real(T'*G_dat);

 k = TtT \ TtG; % O.L.S. fit is a better initial guess, even though infeasible, k<0

 MaxIter = 20;                   % usually enough
 cvg_hst = zeros(2*n,MaxIter);   % convergence of coefficients and multipliers

 for iter = 1:MaxIter            % --- Start Main Loop

    A   = find(k < 2*eps); l = length(A);   % active set for update constraints
    % Ia is the constraint gradient w.r.t. the step vector h
    Ia = zeros(l,n); for i=1:l, Ia(i,A(i)) = 1; end

    % KKT equations
    lambda = zeros(n,1);                        % Lagrange multiplier
    XTX = [ TtT    Ia'      ;                   % dL / dh
            Ia   zeros(l,l) ];                  % dL / d lambda

    XTY = [ -TtT*k + TtG - alpha ;              % dL / dh
            -k(A)                ];             % dL / d lambda

    h_lambda = XTX \ XTY;                       % solve the system

%

    h = h_lambda(1:n);                          % the step
    lambda(A) = h_lambda(n+1:end);              % the non-zero multipliers

   % if an element of k+h becomes negetive, reduce the length of step h to dh*h
   dh = 1;
   [h_test_min, idx] = min(k+h);
   if h_test_min < 0
                   dh = -k(idx)/h(idx);
   end

```

```
    k = (k  +  dh * h);                              % update the Prony coefficients

    figure(102)                                      % plot msmnt points and fit
     G_hat = T*k;
     clf
     subplot(211)
     semilogx ( w,real(G_dat),'or', w,real(G_hat),'-k')
      ylabel('storage modulus,  G''(\omega) ')
      legend('G''(\omega) meas.','G''(\omega) fit','location','northwest')
     subplot(212)
     semilogx ( w,imag(G_dat),'ob', w,imag(G_hat),'-k')
      xlabel('\omega, rad/s')
      ylabel('loss modulus, G"(\omega) ')
      legend('G"(\omega) meas.','G"(\omega) fit','location','northwest')
     drawnow

    cvg_hst(:,iter) = [ k ; lambda ];                      % convergence history
    if ( norm(h) < norm(k)/1e3 && min(k) > -5*eps )       % convergence check
        break;
    end

 end                              % --- End Main Loop

  cvg_hst = cvg_hst(:,1:iter);

% asymptotic standard errors of the Prony coefficients ???
% k_std_err = sqrt(norm(G_dat-T*k)/(m-n+1) * diag(real(inv(TtTT))));

 ko = k(1);
 k = k(2:n);

% ---------------------------------------------------------------------- PRONY_FIT
%                                                          HP Gavin, 2013-10-04
```