

All the following is subject to  $\mathbf{w}, \mathbf{s} \geq 0$ :

$$\begin{aligned}
\mathcal{L} &= \min_{\mathbf{w}, \mathbf{s}} ||M\mathbf{w}||^2 + \mu ||\mathbf{1} - A\mathbf{w} - \mathbf{s}||^2 \\
&= \min_{\mathbf{w}, \mathbf{s}} \mathbf{w}^T M^T M \mathbf{w} + \mu ((\mathbf{1}^T - \mathbf{w}^T A^T - \mathbf{s}^T)(\mathbf{1} - A\mathbf{w} - \mathbf{s})) \\
&= \min_{\mathbf{w}, \mathbf{s}} \mathbf{w}^T M^T M \mathbf{w} + \mu (\mathbf{1}^T \mathbf{1} - \mathbf{1}^T A \mathbf{w} - \mathbf{1}^T \mathbf{s} - \mathbf{w}^T A^T \mathbf{1} + \mathbf{w}^T A^T A \mathbf{w} + \mathbf{w}^T A^T \mathbf{s} - \mathbf{s}^T \mathbf{1} + \mathbf{s}^T A \mathbf{w} + \mathbf{s}^T \mathbf{s}) \\
&= \min_{\mathbf{w}, \mathbf{s}} \mathbf{w}^T (M^T M + \mu A^T A) \mathbf{w} + \mu \mathbf{s}^T I^T I \mathbf{s} + \mu (1 - 2\mathbf{1}^T A \mathbf{w} - 2\mathbf{1}^T \mathbf{s} + 2\mathbf{w}^T A^T \mathbf{s}) \\
&= \min_{\mathbf{y}} \mathbf{y}^T \underbrace{\begin{pmatrix} M^T M + \mu A^T A & \mu A^T \\ \mu A & \mu I \end{pmatrix}}_{C^T C} \mathbf{y} - 2 \underbrace{\begin{pmatrix} \mu \mathbf{1}^T A \\ \mu \mathbf{1}^T \end{pmatrix}}_{\mathbf{d}^T} \mathbf{y} + \underbrace{\mu \mathbf{1}^T \mathbf{1}}_{\mathbf{d}^T \mathbf{d}} \\
&= \min_{\mathbf{y}} \mathbf{y}^T H \mathbf{y} + \mathbf{f} \mathbf{y}
\end{aligned}$$

where  $\mathbf{y}$  is the  $m + n$  vector  $\begin{pmatrix} \mathbf{w} \\ \mathbf{s} \end{pmatrix} \geq 0$ . Yet it still does not look like:

$$\min_{\mathbf{y}} ||C\mathbf{y} - \mathbf{d}||^2 = \min_{\mathbf{y}} \mathbf{y}^T C^T C \mathbf{y} - 2\mathbf{d}^T C \mathbf{y} + \mathbf{d}^T \mathbf{d}$$

because of  $M$ .

Listing 1: Solving minimization problem with the subset method

```

function [w, Aw, L] = compute_graph(X, kind, mu)
[n, d] = size(X);
m = nchoosek(n, 2);
M = sparse(d*n, m);
U = sparse(n, m);
w = [];
MAX_ITER = 50;
nb_iter = 0;
bin_lower = n*(0:n-1) - cumsum(0:n-1);
considered_last_time = [];

% At the end, we cannot have more than  $\frac{d+1}{n}$  edges according to
% Theorem 3.1. But we must start with only a small subset of them. So we first
% select randomly 7% of them (for no specific reason but cinematographic
% one). Actually, it may be more sensitive to use some kind of heuristic like
% nearest neighbors at this stage to be more efficient later.

edges = randi(m, 1, floor(0.33*(d+1)*n));

while (numel(edges) > 0 && nb_iter < MAX_ITER)
    % Then we update the corresponding element (i,j) = e of U with
    % respectively 1 and -1.
    vertex_i = arrayfun(@(x) find(x' <= bin_lower, 1, 'first'), edges) - 1;

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vertex_j = vertex_i + edges - bin_lower(vertex_i);
positive = bsxfun (@(x,y) sub2ind(size(U), x, y), vertex_i, edges);
negative = bsxfun (@(x,y) sub2ind(size(U), x, y), vertex_j, edges);
U(positive) = 1;
U(negative) = -1;
A = abs(U);
assert(sum(A(:))/2 <= (d+1)*n, 'there are too many edges');

T = U'*X; %  $y^{(k)} = U^T x^k$  is thus the  $k$ th column of  $T$ 
% TODO: use parfor
for k=1:d
    first_row = 1 + (k-1)*n;
    last_row = n + (k-1)*n;
    Yk = spdiags(T(:,k), [0], m, m);
    M(first_row:last_row, :) = U*Yk;
end
% Now that we have built our matrices, we can solve the minimization problem
% TODO use SDPT3, although the documentation is quite intimidating:
% http://www.math.nus.edu.sg/~mattohkc/sdpt3/guide4-0-draft.pdf
% It would be especially usefull as MATLAB seems to convert  $M'*M$  to
% a full matrice, which takes around  $2n^4$  bytes of memory (so 8GB for
%  $n = 250$ ).
if strcmpi(kind, 'hard')
    % we only want to constrain the nodes that have edges to be of
    % degree at least 1.
    o = optimoptions(@quadprog, 'Algorithm', 'active-set', 'Display', 'final-detailed');
    [w, f, flag, output, lambda] = quadprog(M'*M, sparse(m, 1), -A, -(sum(A, 2)>0), [], [], [], [], w, o);
    z = lambda.ineqlin;
    derivative = 2*M'*M*w - A'*z;
    save('out', 'M', 'w', 'A', 'lambda', 'derivative');
else
    % According to the paper, we want to solve
    %  $\min_{w,s} ||Mw||^2 + \mu ||1 - Aw - s||$ 
    % subject to  $w, s \geq 0$ , but I don't see how to formulate that for
    % quadprog or lsqnonneg (see http://math.stackexchange.com/q/545280)
    error(strcat(kind, ' is not yet implemented'));
end
end
[val, may_be_added]=sort(derivative(find(derivative<0)));
if ((length(may_be_added) == 0) || (length(may_be_added) == length(
    considered_last_time) && all(may_be_added' == considered_last_time)))
    break;
end
end
% The paper says: we add to our quadratic program the edges with the smallest
%  $\frac{d\Lambda}{dw_{i,j}}$  values, which I think mean not all. For now,
% let's take half of them. TODO take only the one below average or look at
% diff.

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edges = may_be_added(1:max(1, floor(end/2)))';
considered_last_time = may_be_added;
nb_iter = nb_iter + 1;
end
Aw = A*w;
W = spdiags(w, [0], m, m);
L = U*W*U';
end

```

Listing 2: Computing hard graph

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function [w, Aw, L] = compute_hard_graph(X)
[w, Aw, L] = compute_graph(X, 'hard');
end

```

Listing 3: Computing  $\alpha$ -soft graph

```

function [w, Aw, L] = compute_alpha_graph(X, alpha, tol)
[n, d] = size(X);
m = nchoosek(n, 2);
mu = 5*rand();
tau0 = 1.5;
MAX_ITER = 50;
% Set  $\lambda$  so that  $\tau \geq 1$  with equality at MAX_ITER.
lambda = (tau0 - 1)/MAX_ITER;
can_improve = true;
while (can_improve)
    w, Aw, L = compute_graph(X, 'soft', mu);
    tmp = max(zeros(m, 1), ones(m, 1) - A*w);
    alpha_bar = tmp'*tmp/n;
    % Maybe we don't need this complication and keep a fixed  $\tau = \tau_0$ .
    tau = tau0/(1 + nb_iter*lambda);
    if (alpha_bar < alpha)
        % We want to increase  $\bar{\alpha}$  so we need decrease  $\mu$ , which in
        % turn require  $\tau \leq 1$ 
        tau = 1/tau;
    end
    % It is supposed to correspond to: "we then adjust  $\mu$  up or down
    % proportionally to how far  $\frac{\eta(w)}{n} = \bar{\alpha}$  is from the
    % desired value of  $\alpha$ ."
    mu = tau*abs(alpha_bar - alpha)/alpha;
    nb_iter = nb_iter + 1;
    can_improve = abs(alpha_bar - alpha) < tol && nb_iter < MAX_ITER;
end
end

```

Listing 4: Use the built graph to classify samples

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function result = graph_classify(labelled, label, unlabelled)
n = numel(label);

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u = size(unlabelled, 1);
X = [labelled; unlabelled];
[w, Aw, L] = compute_hard_graph(X);
beq = [label; zeros(u, 1)];
Aeq = [eye(n) zeros(n, u); zeros(u, n+u)];
% TODO look at the fast method suggested in the paper: Spielman, D. A.,
% Teng, S.-H. (2004). Nearly-linear time algorithms for graph partitioning,
% graph sparsification, and solving linear systems. Proc. 36th ACM STOC.
x = quadprog(L, [], [], [], Aeq, beq);
result = x(n+1:end) > 0.5;
end

```