User Guide for LDL, a concise sparse Cholesky package

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VERSION 2.0.3, Jan 25, 2011

Abstract

The LDL software package is a set of short, concise routines for factorizing symmetric positive-definite sparse matrices, with some applicability to symmetric indefinite matrices. Its primary purpose is to illustrate much of the basic theory of sparse matrix algorithms in as concise a code as possible, including an elegant method of sparse symmetric factorization that computes the factorization row-by-row but stores it column-by-column. The entire symbolic and numeric factorization consists of less than 50 lines of code. The package is written in C, and includes a MATLAB interface.

1 Overview

LDL is a set of short, concise routines that compute the \mathbf{LDL}^T factorization of a sparse symmetric matrix \mathbf{A} . Its primary purpose is to illustrate much of the basic theory of sparse matrix algorithms in as compact a code as possible, including an elegant method of sparse symmetric factorization (related to [9, 11]). The lower triangular factor \mathbf{L} is computed rowby-row, in contrast to the conventional column-by-column method. Although it does not achieve the same level of performance as methods based on dense matrix kernels (such as [12, 13]), its performance is competitive with column-by-column methods that do not use dense kernels [4, 5, 6].

Section 2 gives a brief description of the algorithm used in the symbolic and numeric factorization. A more detailed tutorial-level discussion may be found in [14]. Details of the concise implementation of this method are given in Section 3. Sections 4 and 5 give an overview of how to use the package in MATLAB and in a stand-alone C program.

2 Algorithm

The underlying numerical algorithm is described below. The kth step solves a lower triangular system of dimension k-1 to compute the kth row of **L** and the d_{kk} entry of the

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diagonal matrix **D**. Colon notation is used for submatrices. For example, $\mathbf{L}_{k,1:k-1}$ refers to the first k-1 columns of the kth row of **L**. Similarly, $\mathbf{L}_{1:k-1,1:k-1}$ refers to the leading (k-1)-by-(k-1) submatrix of **L**.

```
Algorithm 1 (LDL<sup>T</sup> factorization of a n-by-n symmetric matrix A)
```

```
for k = 1 to n

(step 1) Solve \mathbf{L}_{1:k-1,1:k-1}\mathbf{y} = \mathbf{A}_{1:k-1,k} for \mathbf{y}

(step 2) \mathbf{L}_{k,1:k-1} = (\mathbf{D}_{1:k-1,1:k-1}^{-1}\mathbf{y})^{\mathsf{T}}

(step 3) l_{kk} = 1

(step 4) d_{kk} = a_{kk} - \mathbf{L}_{k,1:k-1}\mathbf{y}

end for
```

The algorithm computes an \mathbf{LDL}^T factorization without numerical pivoting. It can thus factorize any symmetric positive definite matrix, and any symmetric indefinite matrix whose leading minors are all well-conditioned.

When **A** and **L** are sparse, step 1 of Algorithm 1 requires a triangular solve of the form $\mathbf{L}\mathbf{x} = \mathbf{b}$, where all three terms in the equation are sparse. This is the most costly step of the Algorithm. Steps 2 through 4 are fairly straightforward.

Let \mathcal{X} and \mathcal{B} refer to the set of indices of nonzero entries in \mathbf{x} and \mathbf{b} , respectively, in the lower triangular system $\mathbf{L}\mathbf{x} = \mathbf{b}$. To compute \mathbf{x} efficiently the nonzero pattern \mathcal{X} must be found first. In the general case when \mathbf{L} is arbitrary [8], the nonzero pattern \mathcal{X} is the set of nodes reachable via paths in the graph G_L from all nodes in the set \mathcal{B} , and where the graph G_L has n nodes and a directed edge (j,i) if and only if l_{ij} is nonzero. To compute the numerical solution to $\mathbf{L}\mathbf{x} = \mathbf{b}$ by accessing the columns of \mathbf{L} one at a time, \mathcal{X} can be traversed in any topological order of the subgraph of G_L consisting of nodes in \mathcal{X} . That is, x_j must be computed before x_i if there is a path from j to i in G_L . The natural order $(1, 2, \ldots, n)$ is one such ordering, but that requires a costly sort of \mathcal{X} . With a graph traversal and topological sort, the solution of $\mathbf{L}\mathbf{x} = \mathbf{b}$ can be computed using Algorithm 2 below. The computation of \mathcal{X} and \mathbf{x} both take time proportional to the floating-point operation count.

Algorithm 2 (Solve Lx = b, where L is lower triangular with unit diagonal)

```
\mathcal{X} = \operatorname{Reach}_{G_L}(\mathcal{B})

\mathbf{x} = \mathbf{b}

for i \in \mathcal{X} in any topological order

\mathbf{x}_{i+1:n} = \mathbf{x}_{i+1:n} - \mathbf{L}_{i+1:n,i}x_i

end for
```

The general result also governs the pattern of \mathbf{y} in Algorithm 1. However, in this case \mathbf{L} arises from a sparse Cholesky factorization, and is governed by the elimination tree [10]. A general graph traversal is not required. In the elimination tree, the parent of node i is the smallest j > i such that l_{ji} is nonzero. Node i has no parent if column i of \mathbf{L} is completely zero below the diagonal; i is a root of the elimination tree in this case. The nonzero pattern of \mathbf{x} is the union of all the nodes on the paths from any node i (where b_i is nonzero) to the root of the elimination tree [9, Thm 2.4]. It is referred to here as a tree, but in general it can be a forest.

Rather than a general topological sort of the subgraph of G_L consisting nodes reachable from nodes in \mathcal{B} , a simpler tree traversal can be used. First, select any nonzero entry b_i and

follow the path from i to the root of tree. Nodes along this path are marked and placed in a stack, with i at the top of the stack and the root at the bottom. Repeat for every other nonzero entry in b_i , in arbitrary order, but stop just before reaching a marked node (the result can be empty if i is already in the stack). The stack now contains \mathcal{X} , a topological ordering of the nonzero pattern of \mathbf{x} , which can be used in Algorithm 2 to solve $\mathbf{L}\mathbf{x} = \mathbf{b}$. The time to compute \mathcal{X} using an elimination tree traversal is much faster than the general graph traversal, taking time proportional to the size of \mathcal{X} rather than the number of floating-point operations required to compute \mathbf{x} .

In the kth step of the factorization, the set \mathcal{X} becomes the nonzero pattern of row k of \mathbf{L} . This step requires the elimination tree of $\mathbf{L}_{1:k-1,1:k-1}$, and must construct the elimination tree of $\mathbf{L}_{1:k,1:k}$ for step k+1. Recall that the parent of i in the tree is the smallest j such that i < j and $l_{ji} \neq 0$. Thus, if any node i already has a parent j, then j will remain the parent of i in the elimination trees of all other larger leading submatrices of \mathbf{L} , and in the elimination tree of \mathbf{L} itself. If $l_{ki} \neq 0$ and i does not have a parent in the elimination tree of $\mathbf{L}_{1:k-1,1:k-1}$, then the parent of i is k in the elimination tree of $\mathbf{L}_{1:k,1:k}$. Node k becomes the parent of any node $i \in \mathcal{X}$ that does not yet have a parent.

Since Algorithm 2 traverses \mathbf{L} in column order, \mathbf{L} is stored in a conventional sparse column representation. Each column j is stored as a list of nonzero values and their corresponding row indices. When row k is computed, the new entries can be placed at the end of each list. As a by-product of computing \mathbf{L} one row at a time, the columns of \mathbf{L} are computed in a sorted manner. This is a convenient form of the output. MATLAB requires the columns of its sparse matrices to be sorted, for example. Sorted columns improve the speed of Algorithm 2, since the memory access pattern is more regular. The conventional column-by-column algorithm [4, 5] does not produce columns of \mathbf{L} with sorted row indices.

A simple symbolic pre-analysis can be obtained by repeating the subtree traversals. All that is required to compute the nonzero pattern of the kth row of \mathbf{L} is the partially constructed elimination tree and the nonzero pattern of the kth column of \mathbf{A} . This is computed in time proportional to the size of this set, using the elimination tree traversal. Once constructed, the number of nonzeros in each column of \mathbf{L} is incremented, for each entry in \mathcal{X} , and then \mathcal{X} is discarded. The set \mathcal{X} need not be constructed in topological order, so no stack is required. The run time of the symbolic analysis algorithm is thus proportional to the number of nonzeros in \mathbf{L} . This is more costly than the optimal algorithm [7], which takes time essentially proportional to the number of nonzeros in \mathbf{A} . The memory requirements are just the matrix \mathbf{A} and a few size-n integer arrays. The result of the algorithm is the elimination tree, a count of the number of nonzeros in each column of \mathbf{L} , and the cumulative sum of the column counts.

3 Implementation

Because of its simplicity, the implementation of this algorithm leads to a very short, concise code. The symbolic analysis routine ldl_symbolic shown in Figure 1 consists of only 18 lines of executable C code. This includes 5 lines of code to allow for a sparsity-preserving ordering **P** so that either **A** or **PAP**^T can be analyzed, 3 lines of code to compute the cumulative sum of the column counts, and one line of code to speed up a for loop. An additional line

of code allows for a more general form of the input sparse matrix A.

The n-by-n sparse matrix A is provided in compressed column form as an int array Ap of length n+1, an int array Ai of length nz, and a double array Ax also of length nz, where nz is the number of entries in the matrix. The numerical values of entries in column j are stored in $Ax[Ap[j] \dots Ap[j+1]-1]$ and the corresponding row indices are in $Ai[Ap[j] \dots Ap[j+1]-1]$. With Ap[0] = 0, the number of entries in the matrix is nz = Ap[n]. If no fill-reducing ordering P is provided, only entries in the upper triangular part of A are considered. If P is provided and row/column i of the matrix A is the k-th row/column of PAP^T , then P[k]=i. Only entries in the upper triangular part of PAP^T are considered. These entries may be in the lower triangular part of A, so to ensure that the correct matrix is factorized, all entries of A should be provided when using the permutation input P.

The outputs of ldl_symbolic are three size-n arrays: Parent holds the elimination tree, Lnz holds the counts of the number of entries in each column of L, and Lp holds the cumulative sum of Lnz. The size-n array Flag is used as workspace. None of the output or workspace arrays need to be initialized.

The ldl_numeric numeric factorization routine shown in Figure 2 consists of only 31 lines of executable code. It includes this same subtree traversal algorithm as ldl_symbolic, except that each path is placed on a stack that holds nonzero pattern of the kth row of \mathbf{L} . This traversal is followed by a sparse forward solve using this pattern, and all of the nonzero entries in the resulting kth row of \mathbf{L} are appended to their respective columns in the data structure of \mathbf{L} .

After the matrix is factorized, the ldl_lsolve, ldl_dsolve, and ldl_ltsolve routines shown in Figure 3 are provided to solve $\mathbf{L}\mathbf{x} = \mathbf{b}$, $\mathbf{D}\mathbf{x} = \mathbf{b}$, and $\mathbf{L}^\mathsf{T}\mathbf{x} = \mathbf{b}$, respectively. Together, they solve $\mathbf{A}\mathbf{x} = \mathbf{b}$, and consist of only 10 lines of executable code. If a fill-reducing permutation is used, ldl_perm and ldl_permt must be used to permute \mathbf{b} and \mathbf{x} accordingly.

In addition to appearing as a Collected Algorithm of the ACM [3], LDL is available at http://www.cise.ufl.edu/research/sparse.

4 Using LDL in MATLAB

The simplest way to use LDL is within MATLAB. Once the ldlsparse mexFunction is compiled and installed, the MATLAB statement [L, D, Parent, f1] = ldlsparse (A) returns the sparse factorization A = (L+I)*D*(L+I)', where L is lower triangular, D is a diagonal matrix, and I is the n-by-n identity matrix (ldlsparse does not return the unit diagonal of L). The elimination tree is returned in Parent. If no zero on the diagonal of D is encountered, f1 is the floating-point operation count. Otherwise, D(-f1,-f1) is the first zero entry encountered. Let d=-f1. The function returns the factorization of A (1:d,1:d), where rows d+1 to n of L and D are all zero. If a sparsity preserving permutation P is passed, [L, D, Parent, f1] = ldlsparse (A,P) operates on A(P,P) without forming it explicitly.

The statement x = 1dlsparse (A, [], b) is roughly equivalent to $x = A \setminus b$, when A is sparse, real, and symmetric. The LDL^T factorization of A is performed. If P is provided, x = 1dlsparse (A, P, b) still performs $x = A \setminus b$, except that A(P,P) is factorized instead.

Figure 1: ldl_symbolic: finding the elimination tree and column counts

```
void ldl_symbolic
                        /* A and L are n-by-n, where n >= 0 */
    int n,
    int Ap [],
                        /* input of size n+1, not modified */
    int Ai [],
                        /* input of size nz=Ap[n], not modified */
                        /* output of size n+1, not defined on input */
    int Lp [],
                        /* output of size n, not defined on input */
    int Parent [],
                        /* output of size n, not defined on input */
    int Lnz [],
    int Flag [ ],
                        /* workspace of size n, not defn. on input or output */
                        /* optional input of size n */
    int P [ ],
    int Pinv [ ]
                        /* optional output of size n (used if P is not NULL) */
   int i, k, p, kk, p2;
    if (P)
        /* If P is present then compute Pinv, the inverse of P */
        for (k = 0; k < n; k++)
        {
           Pinv [P [k]] = k ;
   }
    for (k = 0 ; k < n ; k++)
        /* L(k,:) pattern: all nodes reachable in etree from nz in A(0:k-1,k) */
        Parent [k] = -1;
                                   /* parent of k is not yet known */
                                    /* mark node k as visited */
        Flag [k] = k;
        Lnz [k] = 0;
                                    /\ast count of nonzeros in column k of L \ast/
        kk = (P) ? (P [k]) : (k) ; /* kth original, or permuted, column */ \,
        p2 = Ap [kk+1];
        for (p = Ap [kk] ; p < p2 ; p++)
            /* A (i,k) is nonzero (original or permuted A) */
            i = (Pinv) ? (Pinv [Ai [p]]) : (Ai [p]) ;
            if (i < k)
                /* follow path from i to root of etree, stop at flagged node */
                for ( ; Flag [i] != k ; i = Parent [i])
                    /* find parent of i if not yet determined */
                    if (Parent [i] == -1) Parent [i] = k;
                    Lnz [i]++ ;
                                                        /* L (k,i) is nonzero */
                                                        /* mark i as visited */
                    Flag [i] = k;
           }
        }
   }
    /* construct Lp index array from Lnz column counts */
   Lp [0] = 0 ;
   for (k = 0 ; k < n ; k++)
        Lp [k+1] = Lp [k] + Lnz [k] ;
}
```

Figure 2: ldl_numeric: numeric factorization

```
/* returns n if successful, k if D (k,k) is zero */
int ldl_numeric
                       /* A and L are n-by-n, where n >= 0 */
    int n,
                        /* input of size n+1, not modified */
    int Ap [],
    int Ai [],
                       /* input of size nz=Ap[n], not modified */
    double Ax [],
                       /* input of size nz=Ap[n], not modified */
                       /* input of size n+1, not modified */
    int Lp [],
    int Parent [ ],
                       /* input of size n, not modified */
   int Lnz [],
                       /* output of size n, not defn. on input */
    int Li [],
                       /* output of size lnz=Lp[n], not defined on input */
    double Lx [],
                       /* output of size lnz=Lp[n], not defined on input */
                       /* output of size n, not defined on input */
   double D [],
    double Y [ ],
                       /* workspace of size n, not defn. on input or output */
    int Pattern [],
                       /* workspace of size n, not defn. on input or output */
                       /* workspace of size n, not defn. on input or output */
   int Flag [ ],
   int P [ ],
                       /* optional input of size n */
                       /* optional input of size n */
   int Pinv [ ]
   double yi, l_ki ;
    int i, k, p, kk, p2, len, top;
   for (k = 0; k < n; k++)
        /* compute nonzero Pattern of kth row of L, in topological order */
       Y [k] = 0.0;
                                   /* Y(0:k) is now all zero */
                                   /* stack for pattern is empty */
       top = n ;
       Flag [k] = k;
                                   /* mark node k as visited */
       Lnz [k] = 0:
                                   /* count of nonzeros in column k of L */
       kk = (P) ? (P [k]) : (k) ; /* kth original, or permuted, column */
       p2 = Ap [kk+1];
       for (p = Ap [kk] ; p < p2 ; p++)
           i = (Pinv) ? (Pinv [Ai [p]]) : (Ai [p]) ; /* get A(i,k) */
           if (i <= k)
               Y [i] += Ax [p] ; /* scatter A(i,k) into Y (sum duplicates) */
               for (len = 0 ; Flag [i] != k ; i = Parent [i])
               {
                   Pattern [len++] = i ; /* L(k,i) is nonzero */
                   Flag [i] = k;
                                           /* mark i as visited */
               while (len > 0) Pattern [--top] = Pattern [--len] ;
           }
        /* compute numerical values kth row of L (a sparse triangular solve) */
       D[k] = Y[k];
                                   /* get D(k,k) and clear Y(k) */
       Y [k] = 0.0;
       for (; top < n; top++)
                                   /* Pattern [top:n-1] is pattern of L(:,k) */
            i = Pattern [top] ;
           yi = Y [i] ;
                                   /* get and clear Y(i) */
            Y [i] = 0.0;
           p2 = Lp [i] + Lnz [i] ;
           for (p = Lp [i] ; p < p2 ; p++)
               Y [Li [p]] -= Lx [p] * yi;
           l_ki = yi / D [i] ;
                                   /* the nonzero entry L(k,i) */
            D[k] = 1_{ki} * yi;
           Li [p] = k;
                                   /* store L(k,i) in column form of L */
           Lx [p] = l_ki ;
           Lnz [i]++ ;
                                    /* increment count of nonzeros in col i */
       if (D [k] == 0.0) return (k);
                                           /* failure, D(k,k) is zero */
   return (n);
                      /* success, diagonal of D is all nonzero */
```

Figure 3: Solve routines

```
void ldl_lsolve
    int n,
                         /* L is n-by-n, where n >= 0 */
    double X [ ],
                         /* size n. right-hand-side on input, soln. on output */
    int Lp [],
                         /* input of size n+1, not modified */
    int Li [],
                         /* input of size lnz=Lp[n], not modified */
                         /* input of size lnz=Lp[n], not modified */
    double Lx [ ]
    int j, p, p2 ;
for (j = 0 ; j < n ; j++)</pre>
        p2 = Lp [j+1] ;
        for (p = Lp [j] ; p < p2 ; p++)
            X [Li [p]] -= Lx [p] * X [j] ;
    }
}
void ldl_dsolve
                         /* D is n-by-n, where n >= 0 */
                         /* size n. right-hand-side on input, soln. on output */
/* input of size n, not modified */
    double X [],
    double D [ ]
)
    int j ;
    for (j = 0 ; j < n ; j++)
        X [j] /= D [j] ;
}
void ldl_ltsolve
    int n,
                         /* L is n-by-n, where n >= 0 */
    double X [ ],
                         /\ast size n. right-hand-side on input, soln. on output \ast/
    int Lp [],
                         /* input of size n+1, not modified */
    int Li [],
                         /* input of size lnz=Lp[n], not modified */
                         /* input of size lnz=Lp[n], not modified */
    double Lx [ ]
    int j, p, p2;
    for (j = n-1 ; j \ge 0 ; j--)
        p2 = Lp [j+1] ;
        for (p = Lp [j] ; p < p2 ; p++)
            X [j] -= Lx [p] * X [Li [p]] ;
    }
```

5 Using LDL in a C program

The C-callable LDL library consists of nine user-callable routines and one include file.

- ldl_symbolic: given the nonzero pattern of a sparse symmetric matrix **A** and an optional permutation **P**, analyzes either **A** or **PAP**^T, and returns the elimination tree, the number of nonzeros in each column of **L**, and the Lp array for the sparse matrix data structure for **L**. Duplicate entries are allowed in the columns of **A**, and the row indices in each column need not be sorted. Providing a sparsity-preserving ordering is critical for obtaining good performance. A minimum degree ordering (such as AMD [1, 2]) or a graph-partitioning based ordering are appropriate.
- ldl_numeric: given Lp and the elimination tree computed by ldl_symbolic, and an optional permutation P, returns the numerical factorization of A or PAP^T. Duplicate entries are allowed in the columns of A (any duplicate entries are summed), and the row indices in each column need not be sorted. The data structure for L is the same as A, except that no duplicates appear, and each column has sorted row indices.
- ldl_lsolve: given the factor L computed by ldl_numeric, solves the linear system Lx = b, where x and b are full n-by-1 vectors.
- ldl_dsolve : given the factor **D** computed by $ldl_numeric$, solves the linear system Dx = b.
- ldl_ltsolve: given the factor L computed by ldl_numeric, solves the linear system $\mathbf{L}^{\mathsf{T}}\mathbf{x} = \mathbf{b}$.
- ldl_perm : given a vector **b** and a permutation **P**, returns $\mathbf{x} = \mathbf{Pb}$.
- ldl_permt: given a vector **b** and a permutation **P**, returns $\mathbf{x} = \mathbf{P}^\mathsf{T} \mathbf{b}$.
- ldl_valid_perm: Except for checking if the diagonal of **D** is zero, none of the above routines check their inputs for errors. This routine checks the validity of a permutation **P**.
- ldl_valid_matrix: checks if a matrix **A** is valid as input to ldl_symbolic and ldl_numeric.

Note that the primary input to the ldl_symbolic and ldl_numeric is the sparse matrix **A**. It is provided in column-oriented form, and only the upper triangular part is accessed. This is slightly different than the primary output: the matrix **L**, which is lower triangular in column-oriented form. If you wish to factorize a symmetric matrix **A** for which only the lower triangular part is supplied, you would need to transpose **A** before passing it ldl_symbolic and ldl_numeric.

An additional set of routines is available for use in a 64-bit environment. Each routine name changes uniformly; ldl_symbolic becomes ldl_l_symbolic, and each int parameter becomes type UF_long. The UF_long type is long, except for Microsoft Windows 64, where it becomes __int64.

Figure 4: Example of use

```
#include <stdio.h>
#include "ldl.h"
#define N 10 \, /* A is 10-by-10 */ #define ANZ 19 \, /* # of nonzeros on diagonal and upper triangular part of A */
int main (void)
{
    /* only the upper triangular part of A is required */
           Ap [N+1] = \{0, 1, 2, 3, 4, 6, 7, 9, 11, 15, ANZ]
Ai [ANZ] = \{0, 1, 2, 3, 1,4, 5, 4,6, 4,7, 0,4,7,8, 1,4,6,9\};
                                                                          ANZ},
    double Ax [ANZ] = \{1.7, 1., 1.5, 1.1, .02, 2.6, 1.2, .16, 1.3, .09, 1.6,
                      .13,.52,.11,1.4, .01,.53,.56,3.1},
           \texttt{b} \ [\texttt{N}] \ = \{.287, \ .22, \ .45, \ .44, \ 2.486, \ .72, \ 1.55, \ 1.424, \ 1.621, \ 3.759\};
    double Lx [LNZ], D [N], Y [N];
    int Li [LNZ], Lp [N+1], Parent [N], Lnz [N], Flag [N], Pattern [N], d, i;
    /* factorize A into LDL' (P and Pinv not used) */
    ldl_symbolic (N, Ap, Ai, Lp, Parent, Lnz, Flag, NULL, NULL) ;
    printf ("Nonzeros in L, excluding diagonal: %d\n", Lp [N]) ;
    d = ldl_numeric (N, Ap, Ai, Ax, Lp, Parent, Lnz, Li, Lx, D, Y, Pattern,
        Flag, NULL, NULL);
    if (d == N)
        /* solve Ax=b, overwriting b with the solution x */
        ldl_lsolve (N, b, Lp, Li, Lx);
        ldl_dsolve (N, b, D) ;
        ldl_ltsolve (N, b, Lp, Li, Lx) ;
        for (i = 0 ; i < N ; i++) printf ("x [%d] = %g\n", i, b [i]) ;
    }
    else
    {
        printf ("ldl_numeric failed, D (%d,%d) is zero\n", d, d) ;
    return (0);
}
```

The program in Figure 4 illustrates the basic usage of the LDL routines. It analyzes and factorizes the sparse symmetric positive-definite matrix

and then solves a system $\mathbf{A}\mathbf{x} = \mathbf{b}$ whose true solution is $x_i = i/10$. Note that Li and Lx are statically allocated. Normally they would be allocated after their size, Lp[n], is determined by ldl_symbolic. More example programs are included with the LDL package.

6 Acknowledgments

I would like to thank Pete Stewart for his comments on an earlier draft of this software and its accompanying paper.

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