Automating the generation of algorithms for Generalized Least-Squares problems

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How to efficiently solve...?



... classic problems

•
$$b := \left(X^T X\right)^{-1} X^T y$$



How to efficiently solve...?







How to efficiently solve... ?







How to efficiently solve... ?











$$\bullet \begin{cases} b_{ij} := (X_i^T M_j^{-1} X_i)^{-1} X_i^T M_j^{-1} y_j \\ M_j := h_j \Phi + (1 - h_j) I \end{cases}$$







... sequences of such problems • $\begin{cases} b_{ij} := (X_i^T M_j^{-1} X_i)^{-1} X_i^T M_j^{-1} y_j \\ M_j := h_j \Phi + (1 - h_j) I \end{cases}$ • Smart mapping onto BLAS/LAPACK







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- Smart mapping onto BLAS/LAPACK
- ➡ The decomposition is not unique: many algorithms





Input Matrix equation + App-specific Knowledge



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Input	Matrix equation + App-specific Knowledge
Output	Family of algorithms
Approach	Map onto high-performance kernels



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Search: Not exhaustive. Guidelines. Led by knowledge.





- 2 Automation: Engine
- 3 Automation: Extensions
- 4 Conclusions





How to explore the search space

- Inverse operator:
 - A^{-1} : factorization

$$\blacktriangleright \ LL^T = A, \qquad QR = A, \qquad ZWZ^T = A, \ldots$$



















- Math core:
 - Matrix, Vector, Scalar, Size/Shape, ...
 - Diagonal, L/U triangular, Symm, ...
 - Operators: +, -, *, ⁻¹, ^T. Properties.

• X: {Matrix, FullRank, ColumnPanel} • L: {Matrix, Square, Lower Triangular} • $(LL^T)^{-1} \rightarrow L^{-T}L^{-1}$ • $(X^TX)^{-1} \rightarrow (X^TX)^{-1}$







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$\bullet \ A := X^T X \to A \text{ is SPD}$

• $QR = X \rightarrow Q$ is Orthonormal, R is Triangular







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- Arithmetic, simplifications

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$$(R^T Q^T Q R)^{-1} R^T Q^T$$







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- Arithmetic, simplifications
- Kernels

- Factorizations: QR, LU, Cholesky, Eigen, ...
- BLAS: GEMM, TRSM, GEMV, DOT, ...
- LAPACK: inverse of a triangular matrix, ...
- Extensible



Example: Input



$$\begin{cases} b := (X^T M^{-1} X)^{-1} X^T M^{-1} y \\ M := h \Phi + (1 - h) I \end{cases}$$

```
equation = {
    equal[b,
        times[ inv[ times[ trans[X], inv[M], X ] ],
        ...
        y ]
    ] };
```

```
properties = {
    {X, {"Input", "Matrix", "ColPanel", "FullRank"}}
    {y, {"Input", "Vector" }}
    ...
    {b, {"Output", "Vector" }}
};
```



Example: Generation



$$b := (X^T M^{-1} X)^{-1} X^T M^{-1} y$$



Example: Generation













$$\begin{cases} b_{ij} = (X_i^T M_j^{-1} X_i)^{-1} X_i^T M_j^{-1} y_j & \text{with } 1 \le i \le m \\ M_j = h_j \Phi + (1 - h_j) I & \text{and } 1 \le j \le t. \end{cases}$$

• We have to solve not one but a sequence of correlated problems



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Goal: reuse of computation



Naive approach: for i, for j, ...

f

$$b_{ij} = \left(X_i^T M_j^{-1} X_i\right)^{-1} X_i^T M_j^{-1} y_j$$

or
$$i = 1 : m$$

for $j = 1 : t$
 $LL^T = M_j$
 $X^T \leftarrow X_i^T L^{-T}$
 $QR = X$
 $y \leftarrow L^{-1}y_j$
 $b \leftarrow Q^T y$
 $b_{ij} \leftarrow R^{-1}b$



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Propagating the dependencies

f

$$b_{ij} = \left(X_i^T M_j^{-1} X_i\right)^{-1} X_i^T M_j^{-1} y_j$$

$$\begin{array}{ll} \text{ for } i=1:m \\ \text{ for } j=1:t \\ L_jL_j^T=M_j \\ X_{ij}^T \leftarrow X_i^TL_j^{-T} \\ Q_{ij}R_{ij}=X_{ij} \\ y_j \leftarrow L_j^{-1}y_j \\ b_{ij} \leftarrow Q_{ij}^Ty_j \\ b_{ij} \leftarrow R_{ij}^{-1}b_{ij} \end{array}$$



Loop Transposition

$$b_{ij} = \left(X_i^T M_j^{-1} X_i\right)^{-1} X_i^T M_j^{-1} y_j$$

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$$\begin{array}{l} \text{or } j=1:t\\ \text{for } i=1:m\\ L_jL_j^T=M_j\\ X_{ij}^T\leftarrow X_i^TL_j^{-T}\\ Q_{ij}R_{ij}=X_{ij}\\ y_j\leftarrow L_j^{-1}y_j\\ b_{ij}\leftarrow Q_{ij}^Ty_j\\ b_{ij}\leftarrow R_{ij}^{-1}b_{ij} \end{array}$$

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Reordering

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Computational cost

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How to pick a variant?

• Many algorithms for a single target equation. How do we pick one?



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- Many algorithms for a single target equation. How do we pick one?
- Metric: flop count (often times not too descriptive)

Scenario	Alg. 1	Alg. 2	Alg. 3
One instance	$O(n^3)$	$O(n^3)$	$O(n^3)$
2D sequence	$O(tn^3 + mtn^2)$	$O(tn^3 + mtn^2)$	$O(n^3 + mtn)$



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Elmar Peise, *Hierarchical Performance Modeling for Ranking Dense Linear Algebra Algorithms*, 2012. http://arxiv.org/abs/1207.5217





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- 3 Automation: Extensions





- Domain-specific linear algebra compiler
- $\bullet~$ Equation + Knowledge \rightarrow Families of algorithms



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- Equation + Knowledge \rightarrow Families of algorithms
- Guidelines + Engine
- Extensions: Sequences, cost analysis



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- Sequences of GLSs (GWAS): speedups > 100



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TO-DO

- Encode more available knowledge
- Rank algorithms to pick the "best"
- Matlab/Fortran code generator



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More details in

D. Fabregat, P. Bientinesi, A Domain-Specific Compiler for Linear Algebra Operations, 2012. http://arxiv.org/abs/1205.5975

Further questions?

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