

Query languages with structural and analytic properties

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1 MATLANG syntax and semantics

We assume that we have a supply of matrix variables. The definition of an instance I on MATLANG is a function defined on a nonempty set $var(I) = \{A, B, M, C, \dots\}$, that assigns a concrete matrix to each element (matrix *name*) of $var(I)$.

Every expression e is a matrix, either a matrix of $var(I)$ (*base* matrix, if you will) or a result of an operation over matrices.

The syntax of MATLANG expressions is defined by the following grammar. Every sentence is an expression itself.

$$\begin{aligned}
 e &= M && \text{(matrix variable)} \\
 \text{let } M = e_1 \text{ in } e_2 &&& \text{(local binding)} \\
 e^* &&& \text{(conjugate transpose)} \\
 \mathbf{1}(e) &&& \text{(one-vector)} \\
 \text{diag}(e) &&& \text{(diagonalization of a vector)} \\
 e_1 \cdot e_2 &&& \text{(matrix multiplication)} \\
 \text{apply}[f](e_1, \dots, e_n) &&& \text{(pointwise application of } f)
 \end{aligned}$$

The operations used in the semantics of the language are defined over complex numbers.

- **Transpose:** if A is a matrix then A^* is its conjugate transpose.
- **One-vector:** if A is a $n \times m$ matrix then $\mathbf{1}(A)$ is the $n \times 1$ column vector full of ones.
- **Diag:** if v is a $m \times 1$ column vector then $\text{diag}(v)$ is the matrix

$$\begin{bmatrix}
 v_1 & 0 & 0 & \dots & 0 \\
 0 & v_2 & 0 & \dots & 0 \\
 \dots & \dots & \dots & \dots & \dots \\
 0 & 0 & 0 & \dots & v_m
 \end{bmatrix}$$

- **Matrix multiplication:** if A is a $n \times m$ matrix and B is a $m \times p$ matrix then $A \cdot B$ is the $n \times p$ matrix with $(AB)_{ij} = \sum_{k=1}^n A_{ik}B_{kj}$.
- **Pointwise application:** if $A^{(1)}, \dots, A^{(n)}$ are $m \times p$ matrices, then $\text{apply}[f](A^{(1)}, \dots, A^{(n)})$ is the $m \times p$ matrix C where $C_{ij} = f(A_{ij}^{(1)}, \dots, A_{ij}^{(n)})$.

The formal semantics have a set of rules for an expression e to be valid on an instance I , this is, e succesfully evaluates to a matrix A on the instance I . This success is denoted as $e(I) = A$. Here $I[M := A]$ denotes the instance that is equal to I except that maps M to the matrix A .

Expression	Condition for validity
$(\text{let } M = e_1 \text{ in } e_2)(I) = B$	$e_1(I) = A, e_2(I[M := A]) = B$
$e^*(I) = A^*$	$e(I) = A$
$\mathbf{1}(e)(I) = \mathbf{1}(A)$	$e(I) = A$
$\text{diag}(e)(I) = \text{diag}(A)$	$e(I) = A, A \text{ is a column vector}$
$e_1 \cdot e_2(I) = A \cdot B$	$\# \text{ columns of } A = \# \text{ rows of } B$
$\text{apply}[f](e_1, \dots, e_n)(I) = \text{apply}[f](A_1, \dots, A_n)$	$\forall k, e_k(I) = A \text{ and all } A_k \text{ have the same dimensions}$

For example,

$$\text{let } N = \mathbf{1}(M)^* \text{ in } \text{apply}[c](\mathbf{1}(N)),$$

is an expression, where c denotes the constant function $c : x \rightarrow c$. The result is a 1×1 matrix with c as its entry. This expression is equivalent to $\text{apply}[c](\mathbf{1}(\mathbf{1}(M)^*))$.

An example of what can be computed in MATLANG is the mean of a vector:

$$\begin{aligned} &\text{let } N = \mathbf{1}(v)^* \cdot \mathbf{1}(v) \text{ in} \\ &\text{let } S = v^* \cdot \mathbf{1}(v) \text{ in} \\ &\text{let } R = \text{apply}[\div](S, N) \text{ in } R. \end{aligned}$$

Here, N is the 1×1 matrix with the dimension of v as its entry. S computes the sum of all the entries of v . Finally, in R we store the result of the sum divided by the dimension.

One thing that is worth keeping in mind is that pointwise function application is powerful. With the expression $\text{apply}[f](\cdot)$ one can compute other elemental operations over matrices that can be studied separately, such as:

- Scalar multiplication: we compute $c \cdot A$ as

$$\begin{aligned} &\text{let } C = \text{apply}[c](\mathbf{1}(\mathbf{1}(A)^*)) \text{ in} \\ &\text{let } M = \mathbf{1}(A) \cdot C \cdot \mathbf{1}(A^*)^* \text{ in } \text{apply}[\times](M, A). \end{aligned}$$

- Addition: we compute $A + B$ as

$$\text{let } \text{apply}[+](A, B).$$

- Trace: let

$$m(x, y) = \begin{cases} x & \text{if } x - y > 0 \\ 0 & \text{if } x - y \leq 0 \end{cases}$$

Then we compute the trace of A , $\text{tr}(A)$, as

$$\begin{aligned} &\text{let } I = \text{diag}(\mathbf{1}(A)) \text{ in} \\ &\text{let } B = \text{apply}[-](A, I) \text{ in} \\ &\text{let } C = \text{apply}[m](A, B) \text{ in} \\ &\text{let } T = \text{apply}[+](A, I) \text{ in } \mathbf{1}(A)^* \cdot T \cdot \mathbf{1}(A) \end{aligned}$$

2 Adding canonical vectors to MATLAB

One thing that we cannot do in MATLANG is to obtain a specific entry of a matrix. This entry is expected to be a 1×1 matrix. We can do this by adding the standard unit vectors e_j where

$$e_i = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \rightarrow i\text{-th position}$$

We now show some examples of what can be expressed with this new feature. For illustrative reasons, we assume that all the dimensions are well suited for the corresponding operation.

- Get A_{ij} with $e_i^* \cdot A \cdot e_j$.
- The expression $e_i \cdot e_j^*$ is the matrix that has a 1 in the position i, j and zero everywhere else.
- Given a vector v , the expression $v \cdot e_i^*$ is the matrix

$$\begin{bmatrix} 0 & \cdots & v_1 & \cdots & 0 \\ 0 & \cdots & v_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & v_n & \cdots & 0 \end{bmatrix}$$

- Replace column j of A with zeros: $A(I - e_j \cdot e_j^*)$.
- Replace column j of A with a vector v : $A(I - e_j \cdot e_j^*) + v \cdot e_j^*$.

Note that $I = \text{diag}(\mathbf{1}(A))$ and the sum of matrices can be implemented as $\text{apply}[+](A, B)$.

3 Iterations in MATLAB

It is natural for us to wish for some kind of iteration in MATLANG. There's a lot of matrix procedures and formulas that sums or multiplies results over an operation on the same matrix. Some examples:

- The quantity

$$\sum_{i=0}^n A^i = I + A + A^2 + \dots + A^n$$

it's used a lot in computing inverse or graph theory. This is a sum over the operation power to the i of the matrix A .

- In the LU factorization process the result is

$$A = G_1^{-1}G_2^{-2} \cdots G_n^{-1}U = LU$$

for some upper triangular matrix U and some pivot matrices G_1, \dots, G_n . Note that

$$L = \prod_{i=1}^n G_i^{-1}$$

With this in mind, we introduce the following operators:

- Sum:

$$\sum_{v \in e_1(X)} e_2(X, v)$$

means that, for every column vector v of the matrix $e_1(X)$ do $e_2(X, v)$ and sum the result (pointwise).

- Multiplication:

$$\prod_{v \in e_1(X)} e_2(X, v)$$

means that, for every column vector v_i of the matrix $e_1(X)$ do $e_2(X, v_i)$ and matrix multiply the results R_i as they come up, this is, $R_1 R_2 \cdots R_n$.

Obviously, these operations are valid when the dimentions of the matrices match the wanted operation.

Also, note that the definition is not ambiguous in taking column vectors instead of row vectors, or doing the aggregate matrix multiplication by right, because, if you want to take row vector you just need to do

$$\sum_{v \in e_1(X)^*} e_2(X, v).$$

Or, if you want the result of the aggregate multiplication to be computed in the inverse order, note that, since $(AB)^* = B^* A^*$ we have

$$\prod_{v \in e_1(X)}^{\text{left}} e_2(X, v) = \left(\prod_{v \in e_1(X)} e_2(X, v)^* \right)^*.$$

In general, $e_1(X) = \text{diag}(\mathbf{1}(X)) = I$, so we can iterate over canonical vectors of adequate dimension. So, $\sum_v e(X, v)$ means $\sum_{v \in \text{diag}(\mathbf{1}(X))} e(X, v)$.

Now, let's see what we can do with these new operators.

Determinant

Recall that the determinant is define over permutations, this is

$$\det(A) = \sum_p \sigma(p) a_{1p_1} \cdots a_{np_n},$$

where the sum is taken over the $n!$ permutations of the natural order $(1, 2, \dots, n)$ and

$$\sigma(p) = \begin{cases} +1 & \text{if } p \text{ can be restored to natural order in an even number of steps} \\ -1 & \text{if } p \text{ can be restored to natural order in an odd number of steps} \end{cases}$$

In the case of MATLANG, the permutations are represented as permutation matrices, this is, permutations of the identity. In this context, note that, for a permutation matrix P , we compute $a_{1p_1} \cdots a_{np_n}$ as

$$\prod_v v^* \cdot A \cdot (Pv).$$

See that $a_{ip_i} = v_i^* \cdot A \cdot (Pv_i)$, where v_i is the i -th canonical vector.

We also need to compute $\sigma(P)$, to this end, note that

$$\sigma(P) = (-1)^{\sum_{i < j} \{p_i > p_j\}}.$$

Also, let e_i be the canonical vector with a 1 in its i -th entry and

$$Z = \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 0 & \ddots & \ddots & \vdots \\ \cdots & \cdots & \cdots & 1 \\ 0 & \cdots & \cdots & 0 \end{bmatrix}.$$

Now, note that

$$\mathbf{1}^* Z(e_i - e_j) = \begin{cases} +1 & \text{if } i > j \\ -1 & \text{if } i \leq j \end{cases}$$

So

$$\sigma(P) = \prod_{e_i} \prod_{e_j} \mathbf{1}^* Z(Pe_i - Pe_j).$$

Thus, given we can iterate over permutation matrices, we have

$$\det(A) = \sum_P \left(\prod_{e_i} \prod_{e_j} \mathbf{1}^* Z(Pe_i - Pe_j) \right) \left(\prod_v v^* \cdot A \cdot (Pv) \right).$$

Escalar functions are enough

We have that

- **Pointwise application:** if $A^{(1)}, \dots, A^{(n)}$ are $m \times p$ matrices, then $\text{apply}[f](A^{(1)}, \dots, A^{(n)})$ is the $m \times p$ matrix C where $C_{ij} = f(A_{ij}^{(1)}, \dots, A_{ij}^{(n)})$.

So, given the **sum** operator and the function f , we can compute C in the following way:

$$C = \sum_{v_i} \sum_{v_j} f(v_i^* A^{(1)} v_j, \dots, v_i^* A^{(n)} v_j) \cdot v_i v_j^*$$

Recall that $v_i v_j^*$ is the matrix that has a 1 in the position i, j and zero everywhere else.

Thus, the operator $\text{apply}[f]$ is no longer needed.

For example:

- **Matrix sum:**

$$\sum_{v_i} \sum_{v_j} (v_i^* A^{(1)} v_j + \dots + v_i^* A^{(n)} v_j) \cdot v_i v_j^*$$

- **Matrix pointwise multiplication:**

$$\sum_{v_i} \sum_{v_j} (v_i^* A^{(1)} v_j \times \dots \times v_i^* A^{(n)} v_j) \cdot v_i v_j^*$$

Gaussian elimination

Let A be a matrix and α a scalar. For computing Gaussian elimination we turn our attention in the elementary matrices of the form

$$E = I + \alpha \cdot e_i e_j^*.$$

Note that $E \cdot A$ adds a α -multiple of row i to row j . It is worth noting that $E^{-1} = I - \alpha \cdot e_i e_j^*$.

The key property is that, if A is LU factorizable without any row interchange, then $L = (E_1 \cdots E_k)^{-1} = E_k^{-1} \cdots E_1^{-1}$ for some elementary matrices $E_i = I + \alpha_i \cdot e_i e_j^*$.

4 Connection with logic

We show the expressive power of MATLANG. Let RRA be the class of algebras of binary relations with the operations all, identity, set difference, converse and relational composition. Also, let FO_b^3 denote first-order logic with three variables, equality and infinitely many binary relation symbols. This is, FO_b^3 are FO^3 graph queries.

It is known that the logic captured by RRA is FO_b^3 . Now, we show that RRA can be interpreted into MATLANG, thus the expressive power of MATLANG is at least the same as FO_b^3 .

Let U be a nonempty finite set with n elements (and thus has an enumeration u_1, \dots, u_n). Let $\mathcal{A}^U \in \text{RRA}$, this is

$$\mathcal{A}^U = \langle A, \cup, -, \circ, ^{-1}, I \rangle,$$

where

- $A \subseteq \mathcal{P}(U \times U)$, this is, $\forall R \in A. R \subseteq U \times U$. So A is a set of binary relations over U .
- $\cup, -, \circ, ^{-1}$ denote the operations union, set difference, relational composition and converse, respectively. All of them defined over binary relations.
- I is the constant relation symbol that denotes the set $\{(u, u) : u \in U\}$.

Let $R \in A$. Define M^R a matrix such that

$$M_{ij}^R = \begin{cases} 1 & \text{if } (u_i, u_j) \in R \\ 0 & \text{if } (u_i, u_j) \notin R \end{cases}$$

Note that the MATLANG instance of \mathcal{A} , has $|A|$ matrices with dimensions $|U| \times |U|$. Thus binary relations are represented as adjacency matrices.

We now show how to express the RRA operations in MATLANG.

- **All:** let $R \in A$ be any relation. We express $U \times U$ as $M^{U \times U} = \mathbf{1}(M^R) \cdot \mathbf{1}(M^R)^*$.
- **Identity:** let $R \in A$ be any relation. Then we express the constant relation I as $M^I = \text{diag}(\mathbf{1}(M^R))$.
- **Union:** let $R, S \in A$. Then $M^{R \cup S} = \text{apply}[x \vee y](M^R, M^S)$.
- **Set difference:** let $R, S \in A$. Then $M^{R - S} = \text{apply}[x \vee \neg y](M^R, M^S)$.
- **Converse:** let $R \in A$. Then we express $R^{-1} = \{(u, v) \in U \times U : (v, u) \in R\}$ as $M^{R^{-1}} = (M^R)^*$.

- **Relational composition:** let $R, S \in A$, then $M^{R \circ S} = \text{apply}[x > 0](M^R \cdot M^S)$. Where

$$x > 0 = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$$

Thus RRA can be interpreted into MATLANG, and hence so does FO_b^3 , this is, FO^3 graph queries.

5 Boolean MATLANG

Since we want to do queries over graphs with MATLANG. it is worth to consider the boolean case, this is, when the matrix entries are 1 or 0.

For this purpose, we need to redefine the basic operations of MATLANG if necessary. Note that the only operations that need to be redefined are the matrix multiplication and function application, since the **transpose**, **one-vector** and **diag** of a boolean matrix or vector are boolean matrices or vectors.

- **Matrix multiplication:** if A is a $n \times m$ matrix and B is a $m \times p$ matrix then $A \cdot B$ is a $n \times p$ matrix where $(A \cdot B)_{ij} = \bigvee_{k=1}^m A_{ik} \wedge B_{kj}$.
- **Pointwise application:** if $A^{(1)}, \dots, A^{(n)}$ are $m \times p$ matrices, then $\text{apply}[f](A^{(1)}, \dots, A^{(n)})$ is the $m \times p$ matrix C where $C_{ij} = f(A_{ij}^{(1)}, \dots, A_{ij}^{(n)})$.

Note that in the boolean case we need $f : \{0, 1\} \rightarrow \{0, 1\}$. So, for a fixed n there are finitely many functions to apply: 2^{2^n} . Let's call this set \mathcal{F}_n . This is $|\mathcal{F}_n| = 2^{2^n}$.

Since we are in the boolean case, the following condition holds.

$$\forall f \in \mathcal{F}_n \exists g \in \mathcal{F}_n : f(x_1, \dots, x_n) = \neg g(x_1, \dots, x_n),$$

so we can simulate all 2^{2^n} functions with a subset of \mathcal{F}_n of 2^{2^n-1} functions.

6 Expressions as functions

Another way of looking at expressions in MATLANG is as functions between matrix spaces, this is

$$e : (M_1, \dots, M_k) \rightarrow M,$$

where M, M_1, \dots, M_k are matrix spaces, i.e., $M, M_1, \dots, M_k \in \{\mathcal{M}^{n \times m} : n, m \in \mathbb{N}^+\}$.

Some examples:

- If A is $n \times m$ then

$$\begin{aligned} e(A) = t(A) : \mathcal{M}_{n \times m} &\rightarrow \mathcal{M}_{m \times n} \\ A &\rightarrow A^* \end{aligned}$$

- If A is $n \times m$ then

$$e(A) = \mathbf{1}(A) : \mathcal{M}_{n \times m} \rightarrow \mathcal{M}_{n \times 1}$$

$$A \rightarrow n \text{ times} \left\{ \begin{bmatrix} 1 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{bmatrix} \right.$$

- If v is $n \times 1$ then

$$e(v) = \text{diag}(v) : \mathcal{M}_{n \times 1} \rightarrow \mathcal{M}_{n \times n}$$

$$v \rightarrow \begin{bmatrix} v_1 & 0 & 0 & \dots & 0 \\ 0 & v_2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & v_n \end{bmatrix}$$

- If A is $n \times m$ and B is $m \times p$ then

$$e(A, B) = A \cdot B : \mathcal{M}_{n \times m} \times \mathcal{M}_{m \times p} \rightarrow \mathcal{M}_{n \times p}$$

$$(A, B) \rightarrow A \cdot B$$

- If $A^{(1)}, \dots, A^{(n)}$ are $m \times p$ matrices then

$$e(A^{(1)}, \dots, A^{(n)}) = \text{apply}[f](A^{(1)}, \dots, A^{(n)})$$

has domains

$$\mathcal{M}_{m \times p}^n \rightarrow \mathcal{M}_{m \times p}$$

$$(A^{(1)}, \dots, A^{(n)}) \rightarrow C : C_{ij} = f(A_{ij}^{(1)}, \dots, A_{ij}^{(n)}).$$

We can start to analyze if this functions are increasing, decreasing, boolean, etc. Also, we can study the effects of disturbances on the input in the output of these functions.

7 Core of Matlab and R

MATLAB

The basic operations of MATLAB over matrices are:

- **mldivide**(A, B): returns x such that $Ax = B$.
- **descomposition**(A): returns a decomposition or factorization LU, LDL, QR , Cholesky, etc.
- **inv**(A): returns A^{-1} .
- **multiplication**: compute $A \cdot B$.

- **transpose(A)**: returns A^T .
- **conjugate transpose(A)**: returns A' .
- **matrix power(A, k)**: returns A^k .
- **eigen(A)**: returns the eigenvectors and the eigenvectors matrices of A .
- **funm(A, f)**: returns matrix B with elements $b_{ij} = f(a_{ij})$.
- **crossprod(a, b)**: vectorial product, returns c such that $c \perp a, b$.
- **dotprod(a,b)**: returns $a \cdot b$.
- **diag(v)**: v vector. Returns the following matrix:

$$\begin{bmatrix} v_1 & 0 & 0 & \dots & 0 \\ 0 & v_2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & v_n \end{bmatrix}$$

- **diag(A)**: given matrix A , it returns

$$\begin{bmatrix} a_{11} \\ a_{22} \\ \vdots \\ a_{nn} \end{bmatrix}$$

- **det(A)**: returns the determinant of A .
- **zeros(n, m)**: returns a $n \times m$ matrix full of zeros.
- **ones(n, m)**: returns a $n \times m$ matrix full of ones.
- **A[i, j]**: you can get A_{ij} .

R

The basic operations of the language R over matrices are:

- **A%*%B**: matrix multiplication.
- **A*B**: pointwise multiplication.
- **t(A)**: transpose.
- **diag(v)**: returns the matrix

$$\begin{bmatrix} v_1 & 0 & 0 & \dots & 0 \\ 0 & v_2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & v_n \end{bmatrix}$$

- **diag(A)**: Returns the vector

$$\begin{bmatrix} a_{11} \\ a_{22} \\ \vdots \\ a_{nn} \end{bmatrix}$$

- **diag(k)**: k scalar. It creates the $k \times k$ identity matrix.
- **matrix(k, n, m)**: returns the $n \times m$ matrix, where every entry is equal to k .
- **solve(A, b)**: returns x such that $Ax = b$.
- **solve(A)**: returns A^{-1} .
- **det(A)**: determinant of A .
- **y<-eigen(A)**: stores the eigenvalues of A in `y$val` and the eigenvectors in `y$vec`.
- **y<-svd(A)**: it computes and stores the following:
 - `y$d`: vector of the singular values of A .
 - `y$u`: matrix of the left singular vectors of A .
 - `y$v`: matrix of the right singular vectors of A .
- **R<-chol(A)**: Cholesky factorization, $R'R = A$.
- **y<-qr(A)**: QR decomposition, stored in `y$qr`.
- **cbind(A,B, v, ...)**: joins matrices and vector horizontally, returns a matrix.
- **rbind(A,B, v, ...)**: joins matrices and vector vertically, returns a matrix.
- **rowMeans(A)**: returns the vector of the averages over the rows of A .
- **colMeans(A)**: returns the vector of the averages over the columns of A .
- **rowSums(A)**: returns the vector of the sums over the rows of A .
- **colSums(A)**: returns the vector of the sums over the columns of A .
- **outer(A, B, f)**: applies $f(\cdot, \cdot)$. Returns matrix C of entries $c_{ij} = f(a_{ij}, b_{ij})$.
- **A[i, j]**: you can get A_{ij} .