Auto-Differentiating Linear Algebra

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Abstract

Development systems for deep learning, such as Theano, Torch, TensorFlow, or MXNet, are easy-to-use tools for creating complex neural network models. Since gradient computations are automatically baked in, and execution is mapped to high performance hardware, these models can be trained end-to-end on large amounts of data. However, it is currently not easy to implement many basic machine learning primitives in these systems (such as Gaussian processes, least squares estimation, principal components analysis, Kalman smoothing), mainly because they lack efficient support of linear algebra primitives as differentiable operators. We detail how a number of matrix decompositions (Cholesky, LQ, symmetric eigen) can be implemented as differentiable operators. We have implemented these primitives in MXNet, running on CPU and GPU in single and double precision. We sketch use cases of these new operators, learning Gaussian process and Bayesian linear regression models. Our implementation is based on BLAS/LAPACK APIs, for which highly tuned implementations are available on all major CPUs and GPUs.

1 Introduction

Deep neural networks, trained on vast amounts of data, have recently revolutionized several machine learning applications, ranging from object classification and detection in computer vision over large vocabulary speech recognition to machine translation of natural language text. Apart from large amounts of data and high-performance computing hardware, a major driver of this success has been the flexibility and ease of use of modern deep learning development systems (DLDS), such as Theano, Torch, TensorFlow, or MXNet. These systems map algorithms to computation graphs, where nodes are multi-dimensional arrays, and vertices are differentiable operators. Given this abstraction, gradients w.r.t. any node are obtained automatically by way of reverse mode differentiation, a generalization of error backpropagation. While some DLDS maximize flexibility by unfolding the graph on the fly, others may apply graph optimization in order to minimize runtime or memory usage on a specific target hardware. All a user has to do is to specify this symbolic graph, or even just re-combine existing components, and bind it to input data. Not only has this simple means of specifying a complex model lowered the technical bar to entry into cutting-edge ML, it is also dramatically shortening the time from idea to large data experimentation, which is so crucial for data-driven innovation.

Given this massive advance in ease of modeling, it is remarkable to observe how many “pre-deep-learning” algorithmic primitives remain out of reach of current DLDS. Here are some examples, which can be found in any ML standard textbook [4, 2, 7, 9]:

- Least squares estimation, solving linear systems
- Gaussian process models
- Principal components analysis, linear discriminant analysis, canonical correlation analysis
Kalman filtering and smoothing in linear dynamical systems

Why are none of these easily available in most DLDS, as are LSTM or Inception modules? Inspecting the former algorithms, they make use of certain linear algebra primitives, such as Cholesky decomposition, backsubstitution, LQ decomposition, or symmetric eigendecomposition. As we will demonstrate in this work, this limited number of linear algebra primitives is all that is missing in order to cover a substantial number of ML cornerstone algorithms, as long as they are available as differentiable operators.

In this work, we show how the following linear algebra primitives can be incorporated into a DLDS as fully differentiable operators:

- Cholesky decomposition, backsubstitution
- LQ decomposition
- Symmetric eigendecomposition

We contributed implementations for all operators detailed here to the MXNet deep learning development system. Our implementations work both on CPUs and GPUs, and can be used in `float64` or `float32`. We provide a number of concrete examples of how core ML methodology is implemented on top of our novel operators.

There are essentially two ways of including complex linear algebra operators into a DLDS. First, we can re-implement the forward computation in terms of primitives of the DLDS, relying on autograd for backward. Second, we can derive the backward expression, and implement both forward and backward ourselves. The first strategy is often propagated in the automatic differentiation research field, with the final goal of transforming native-language forward code such that gradients are obtained as well. For our work, we chose the latter strategy. While a bit more effort is needed for the derivations, we do not have to re-implement anything difficult, but can instead build on top of existing highly tuned numerical linear algebra software (implementations of BLAS and LAPACK), available for both CPUs and GPUs. As we will demonstrate, this opens the door to incorporating LQ and eigendecomposition into DLDS, robust implementations of which go far beyond of what can be re-implemented with reasonable effort and limited expertise in numerical mathematics.

The structure of this paper is as follows. We summarize related work in Section 2. In Section 3 we sketch several machine learning applications enabled by our novel operators: Gaussian process regression, Bayesian linear regression, and Kalman filtering. Complete example notebooks are available for download, as referenced there. Forward and backward expressions for a range of advanced linear algebra operators are detailed in Section 4, and our implementation of these operators in MXNet is described in Section 5. We close with a discussion.

2 Related Work

We are neither the first to consider reverse mode differentiation for matrix decompositions, nor to include differentiable operators into DLDS. Here, we review related publications and existing code in commonly used DLDS. Note that what we denote backward in the remainder of this work, is called pullback in the automatic differentiation community.

A number of different algorithms for the Cholesky decomposition are proposed in [8]. The backward expression we use here, appears in this work. The author recommends to implement a block version of the operator, for reasons of cache-friendly memory access. However, no code or empirical results are provided. A number of backward expressions for linear algebra are given in [9], among them the one we use for the symmetric eigendecomposition here. The author does not provide code. Also, the non-determinism of eigenvector signs
are not mentioned there. Finally, a number of results for forward and reverse mode differentiation of matrix decompositions are provided in [11]. This work contains pullbacks for the symmetric eigendecomposition (same as ours) and the QR decomposition. For the latter, they concentrate on the case $A = QR \in \mathbb{R}^{m \times n}$, where $m \geq n$, $Q \in \mathbb{R}^{m \times m}$, and $R \in \mathbb{R}^{m \times n}$ is upper triangular and padded with zero rows. In typical machine learning applications, we have $m \gg n$, and an $m \times m$ matrix could not be stored. Their expression is different to ours. They do not provide code. In summary, while most of the backward expressions used in our work here are not strictly novel (a possible exception is our expression for the LQ decomposition), they are not widely known in the ML community. Moreover, none of the work above provides serious implementations on top of standard libraries like BLAS and LAPACK.

2.1 Software

Here, we summarize the current implementations of linear algebra operators in commonly used DLDS. We concentrate on operators which can be first class citizens in a computation graph, because gradients w.r.t. inputs are supported.

We start with TensorFlow [1]. The operators relevant to the current work are `tf.cholesky_` (our `potrf`), `tf.matrix_triangular_solve_` (our `trsm`), and `tf.self_adjoint_eig_` (our `syevd`). Code for backward expressions is at https://github.com/tensorflow/tensorflow/blob/master/tensorflow/python/ops/linalg_grad.py:

- `_CholeskyGrad` (our `potrf_backward`): Implements same expression as ours, but not in-place (three temporary matrices are used).
- `MatrixTriangularSolveGrad` (our `trsm_backward`): Implements same expression as ours.
- `SelfAdjointEigV2Grad` (our `syevd_backward`): Implements same expression as ours, but not in-place (at least three temporary matrices are used).

As discussed in https://github.com/tensorflow/tensorflow/issues/6504, the LQ or QR decomposition is not yet available (an implementation based on [11] is proposed). At a higher level, linear algebra in TensorFlow is mapped to Eigen (eigen.tuxfamily.org). While this simplifies implementations, it is unclear to what extent Eigen supports GPU computation. Moreover, the TensorFlow implementation is not optimized for in-place computations, and a substantial number of temporary matrices are used. It is unclear whether this is due to the dependence on Eigen, or could be fixed.

Another commonly used DLDS is Theano [3]. Here, the relevant operators are `slinalg.Cholesky` (our `potrf`), `slinalg.solve_lower_triangular` (our `trsm`), `nlinalg.Eigh` (our `syevd`). The code is at http://deeplearning.net/software/theano/library/tensor/slinalg.html and http://deeplearning.net/software/theano/library/tensor/nlinalg.html:

- `slinalg.Cholesky.grad` (our `potrf_backward`): Implements the expression from [8], which is related to ours. Not in-place (at least three temporary matrices). Also, the Cholesky factor is recomputed in the backward pass.
- `slinalg.Solve.grad` (our `trsm_backward`): The argument is lower triangular. The implementation is not in-place. Also, the backsubstitution is recomputed in the backward pass.
- `nlinalg.Eigh.grad` (our `syevd_backward`): Channeled through `nlinalg.EighGrad`, which seems to implement an expression related to ours. The computation is certainly not in-place, but employs a for loop. Also, the eigendecomposition is recomputed in the backward pass.

While there is `nlinalg.QRFull` for the QR decomposition, its gradient is not implemented. At a higher level, Theano is calling linear algebra primitives from NumPy and SciPy. These may or may not support GPU computations. The Theano implementation is not optimized for in-place computations, a substantial number
of temporary matrices are used. This fact is quite likely due to the dependence on NumPy and SciPy. A further inefficiency of the Theano backward implementations is that the output of the forward computation is recomputed instead of just being passed. This does not happen in TensorFlow or MXNet.

Finally, there is PyTorch (pytorch.org). The only relevant operator seems to be Potrf (our potrf), whose code is at https://github.com/pytorch/pytorch/blob/master/torch/autograd/_functions/linalg.py. It implements the expression from [8]. The code is quite wasteful, but could be improved (for example, calls to torch.gesv could be replaced by torch.trtrs). Note that while many BLAS and some LAPACK functions are wrapped, most do not have gradients implemented. In summary, too few linear algebra operators are implemented as “first-class citizens” in order to allow for use cases we are interested in there (see Section 5).

The GPFlow project [6] (code at https://github.com/GPflow/GPflow) allows the user to build Gaussian process models on top of TensorFlow [1]. It is using the Cholesky decomposition and backsubstitution operators in TensorFlow, as just discussed. We demonstrate how our operators in MXNet are used to learn Gaussian process models in Section 3.1. Since typical GP applications operate with large dense matrices, it is crucial to avoid unnecessary temporary copies, and a careful in-place implementation such as ours should be advantageous. Also, all our code runs on GPUs and in both float64 and float32. We aim to build Gaussian process methodology on top of MXNet, using our operators. In the context of these developments, comparative studies will be done.

In summary, while some differentiable linear algebra operators are implemented in the most popular DLDS, the support is patchy at best, with TensorFlow being more advanced than others. In general, operators are implemented at a high level, reducing to Eigen (TensorFlow) or NumPy/SciPy (Theano), which may not take full advantage of the underlying execution context (GPU, CPU). Also, not much care is taken to avoid temporary copies. In contrast, we implement our operators into the MXNet core, calling tuned BLAS/LAPACK libraries directly. Most of our operators are implemented in-place, so that no additional memory is required. While this is somewhat more difficult to do (see Section 5), it should pay off in applications such as those in Section 5 where rather large matrices are operated on. We also implement a wider range of operators than others. In particular, we include the LQ factorization, with which least squares estimation can be handled in single precision, whereas the Cholesky decomposition requires double precision.

3 Machine Learning Examples

In this section, we provide some examples for how a small number of linear algebra operators can enable a range of machine learning methodologies inside a DLDS (we make use of MXNet). We focus on code snippets here, complete examples are provided as Jupyter notebooks referenced below.

3.1 Gaussian Processes

Powerful non-parametric regression and classification models are obtained by representing unknown functions by Gaussian processes (GPs). Details about GPs can be found in [8]. Here, we focus on a simple GP regression setup. Suppose we are interested in learning a function \( f(x) \) from data \( \{(x_i, y_i) \mid i = 1, \ldots, n\} \), where \( y_i \in \mathbb{R} \) is a noisy observation of \( f(x_i) \). A GP regression model is obtained by (a) assuming that the function \( f(x) \) is a priori distributed as a Gaussian process with zero mean function and covariance (or kernel) function \( K(x, x') \), and (b) that \( y_i \sim N(f(x_i), \lambda_y) \), namely targets are observed with independent Gaussian noise of variance \( \lambda_y \). The kernel function \( K \) has free hyper-parameters \( \theta \). Given this model, there are two basic problems to be solved. First, we need to learn the hyper-parameters \( \theta \) and \( \lambda_y \). Second, we need to predict mean and variance of \( f(x) \) at test input points \( x_r \). Here, we focus on the harder learning problem. It can conveniently be solved by maximizing the marginal likelihood \( P(y \mid \theta, \lambda_y) \) of the observed data \( y = [y_1, \ldots, y_n]^T \), where the unknown function \( f(\cdot) \) and the noise are integrated out. We show how to express the negative log marginal likelihood \( \phi \) as a symbolic MXNet expression, using the novel operators detailed in Section 4. It is easy to see that

\[
P(y \mid \theta, \lambda_y) = N(y \mid 0, A), \quad A = K + \lambda_y I,
\]
where $K = [K(x_i, x_j)]_{i,j} \in \mathbb{R}^{n \times n}$ is the kernel matrix, and $I \in \mathbb{R}^{n \times n}$ denotes the identity matrix. As derived in [9]:

$$\phi = -\log N(y|0, A) = \frac{1}{2} \left( y^T A^{-1} y + \log|2\pi A| \right).$$

Here, $|X|$ denotes the determinant of an invertible matrix $X$. At this point, we use the Cholesky decomposition (Section 4.2) of $A$:

$$A = LL^T.$$ 

Following [9]:

$$\phi = \frac{1}{2} \left( \|z\|^2 + n \log(2\pi) \right) + \log|L|, \quad z = L^{-1} y.$$

Here is Python code to create an MXNet symbolic expression for $\phi$:

```python
import numpy as np
import mxnet as mx

def gp_regr_criterion_symbol(kern_mat, targets, noise_var, num_cases, dtype=np.float32):
    """Negative log likelihood criterion for Gaussian process regression""
    amat = kern_mat + mx.sym.broadcast_mul(
        mat_eye_symbol(num_cases, dtype),
        mx.sym.reshape(noise_var, shape=(1, 1)))
    chol_fact = mx.sym.linalg.potrf(amat)
    zvec = mx.sym.linalg.trsm(
        chol_fact, mx.sym.reshape(targets, shape=(num_cases, 1)),
        transpose=False, rightside=False)
    sqnorm_z = mx.sym.sum(mx.sym.square(zvec))
    logdet_l = mx.sym.sum(mx.sym.log(mx.sym.abs(
        extract_diag_symbol(chol_fact, num_cases))))
    return 0.5 * (sqnorm_z + (num_cases * np.log(2.0 * np.pi)) + logdet_l)
```

Here, `kern_mat` represents the kernel matrix $K$, `targets` the observed targets $y$, and `noise_var` the noise variance $\lambda_y$. The relevant operators are `linalg.potrf` (compute Cholesky factor $L$ of matrix $A$) and `linalg.trsm` (compute $z = L^{-1} y$). Details for these operators are given in Section 4.2. Since $L$ is a triangular matrix, its log determinant is

$$\log|L| = \log \prod_i l_{ii} = \sum_i \log l_{ii}.$$ 

In the code, `extract_diag_symbol(chol_fact, num_cases)` extracts the diagonal of $L$. Finally, `mat_eye_symbol(num_cases, dtype)` creates the identity matrix of size `num_cases`. `dtype` determines whether computations are done in single or double precision.
Note that the Cholesky factor $L$ is computed once, then used both to compute $z$ and $\log |L|$. In fact, chol_fact represents a single node in the computation graph. Not only does this save memory and compute time, it is also numerically safer than computing the inverse $A^{-1}$ and log determinant $\log |A|$. The complete example code also demonstrates how kernel matrices are computed with linalg.syrk and linalg.gemm2.

Our example shows how hyper-parameter learning in a GP model can be driven by MXNet. While this could well be more efficient than existing GP software packages, the real benefit of inserting GP operators into MXNet lies in the ability to train hybrid models end-to-end. For example, the latent function $f(x)$ could be the sum of a GP and a DNN, or the kernel function $K(x, x')$ could be parameterized in terms of neural networks.

A Jupyter notebook that implements the full GP model based on the above symbolic expression is available at \url{http://github.com/ARCambridge/MXNet_linalg_examples}. In the notebook, we implement the Gaussian (or Radial Basis Function, RBF) kernel, as well as the negative log likelihood criterion for GP regression, as detailed above. We also show how to compute predictive distributions for test points, after hyperparameters have been learned. The notebook is using the GPy framework \url{https://github.com/SheffieldML/GPy} for optimization and plotting, while all computations are done by MXNet executors. In the notebook, we demonstrate hyperparameter learning and prediction on a toy 1D dataset.

### 3.2 Least Squares Estimation. Bayesian Linear Regression

The linear regression problem, also known as least squares estimation, is a cornerstone of applied mathematics. The gold-standard approach to solving the corresponding normal equations is applying the LQ decomposition (or its transpose, the QR decomposition). Here, we focus on Bayesian linear regression \cite{BLR}, which is closely related to the learning criterion is

$$
\phi = -\log P(y) = \frac{1}{2} \left( \log |2\pi \Sigma_y| + y^T \Sigma_y^{-1} y \right).
$$

Define $\alpha := \lambda_w / \lambda_y$. We have that

$$
\log |\Sigma_y| = -n \log(2\pi \lambda_y) = \log |I_n + \alpha X^T X| = \log |M|, \quad M := I_d + \alpha X X^T.
$$

Here, we use a well-known determinant identity. Moreover, the Woodbury identity gives

$$
\Sigma_y^{-1} = \lambda_y^{-1} \left( I_n - \alpha X^T M^{-1} X \right).
$$

Define the matrix

$$
B = [B_1, B_2] \in \mathbb{R}^{d \times (n + d)}, \quad B_1 = I_d, \quad B_2 = \alpha^{1/2} X.
$$

Note that $BB^T = M$. At this point, we use the LQ decomposition:

$$
B = LQ, \quad Q = [Q_1, Q_2], \quad QQ^T = I_d.
$$
Then:
\[ \log |\Sigma_\nu| - n \log(2\pi \lambda_\nu) = \log |M| = \log |LL^T| = 2 \log |L|. \]

Also:
\[ B^T M^{-1} B = Q^T L^T M^{-1} L Q = Q^T Q, \]
so that
\[ \Sigma_\nu^{-1} = \lambda_\nu^{-1} \left( I_n - B_2^T M^{-1} B_2 \right) = \lambda_\nu^{-1} \left( I_n - Q_2^T Q_2 \right). \]

The learning criterion becomes
\[ \phi = \frac{1}{2} \left( 2 \log |L| + n \log(2\pi \lambda_\nu) + \lambda_\nu^{-1} (\|y\|^2 - \|Q_2 y\|^2) \right). \]

Here is Python code to create an MXNet symbolic expression for \( \phi \):

```python
import numpy as np
import mxnet as mx

def bayeslinregr_criterion_symbol(feat_mat, targets, noise_var, prior_var, num_cases, num_dim, dtype=np.float32):
    
    alpha = prior_var / noise_var
    bimat = mx.sym.mat_eye_symbol(num_dim, dtype)
    b2mat = mx.sym.broadcast_mul(feat_mat, mx.sym.reshape(mx.sym.sqrt(alpha), shape=(1, 1)))
    bmat = mx.sym.Concat([bimat, b2mat], dim=1)
    qmat, lmat = mx.sym.linalg.gelqf(bmat)
    ypad = mx.sym.reshape(mx.sym.Concat(
        *[mx.sym.zeros(num_dim, dtype=dtype), targets], dim=0), shape=(num_cases+num_dim, 1))
    tvec = mx.sym.linalg.gemm2(qmat, ypad)
    sqnorm_y = mx.sym.sum(mx.sym.square(targets))
    sqnorm_t = mx.sym.sum(mx.sym.square(tvec))
    logdet_l = mx.sym.sum(mx.sym.log(mx.sym.abs(extract_diag_symbol(lmat, num_dim))))
    return 0.5 * ((sqnorm_y - sqnorm_t) / noise_var + num_cases * (mx.sym.log(noise_var) + np.log(2.0 * np.pi)) + logdet_l)
```
Here, `feat_mat` represents the feature matrix $X$, `targets` the observed targets $y$, `noise_var` the noise variance $\lambda_y$, and `prior_var` the prior variance $\lambda_v$. The relevant operators are `linalg.gelqf` (compute the LQ decomposition $Q, L$ of matrix $B$) and `linalg.gemm2`. The latter computes $Q^T y = Q \hat{y}$, where $\hat{y} = [y^T, \check{y}^T]^T$ is `ypad`. See Section 3.1 for the computation of log $|L|$ (logdet_L).

Note that the BLR learning criterion $\phi$ can also be evaluated using the Cholesky factorization of the matrix $M$. Why is the LQ decomposition needed, whose implementation is more complex? It is well known in numerical linear algebra that the normal equations are solved much more numerically stable by the LQ than the Cholesky factorization, and the same holds for BLR. In the example above, the condition number of $M$ is up to the square of the condition number of $B$. If we use the LQ factorization, $M$ never has to be computed or factorized. This difference is particularly relevant if BLR is used as part of a larger DNN model, where computations are routinely done in single precision (`float32`), to save GPU memory.

Our example shows how hyper-parameter learning in a Bayesian linear regression model can be driven by MXNet. Once more, the real benefit lies in the ability to train hybrid models end-to-end, such as for example DNNs with BLR layers, or BLR with features maps given by DNNs.

A Jupyter notebook that implements the Bayesian linear model based on the above symbolic expression is available at [https://github.com/ARCambridge/MXNet_linalg_examples](https://github.com/ARCambridge/MXNet_linalg_examples). In the notebook, we implement hyperparameter learning and prediction for the BLR model. The notebook is using the `GPy` framework for optimization and plotting, while all computations are done by MXNet executors. We also show how polynomial basis functions can be used as features. A demonstration is done on a toy 1D dataset.

### 3.3 Kalman Filtering

Gaussian linear dynamical systems (LDS) are among the most frequently used models for temporally varying data, with applications in tracking, robotics, control, or acoustic modelling. Inference is analytically tractable, via the Kalman filtering (and smoothing) algorithm. Different to time-varying neural network models, such as LSTMs or GRUs, the Kalman filter propagates distributions over latent states (instead of fixed values), thereby taking uncertainty and errors into account.

The Gaussian LDS is modelling a sequence of `observed` variables $[v_t]$, where $t = 0, 1, \ldots$ indexes time. It makes use of a sequence of `latent` states $h_t$:

$$h_t \sim N(A h_{t-1}, \Sigma_h), \quad v_t \sim N(B h_t, \Sigma_v).$$

Moreover, $h_0 \sim N(\mu_0, \Sigma_0)$. The model parameters are transition matrices $A, B$, covariance matrices $\Sigma_h, \Sigma_v$, as well as $\mu_0, \Sigma_0$. They are learned by maximum likelihood estimation, typically driven by the expectation maximization algorithm, which in turn is powered by Kalman smoothing. In our use case, we fit the Gaussian LDS to a number of time series, and learn parameters by gradient-based optimization. The negative log likelihood is computed by Kalman filtering, which we implement in MXNet.

Full details are provided at [http://gluon.mxnet.io/chapter12_time-series/lds-scratch.html](http://gluon.mxnet.io/chapter12_time-series/lds-scratch.html). Here, we sketch the part which requires our linear algebra operators. The filtering equations $(t-1) \rightarrow t$ are given by

$$\mu_h = A f_{t-1}, \quad \mu_v = B \mu_h, \quad \Sigma_h = AF_{t-1}A^T + \Sigma_h,$$
$$\Sigma_{vv} = B \Sigma_h B^T + \Sigma_v, \quad K_t = \Sigma_h B^T \Sigma_v^{-1},$$
$$f_t = \mu_h + K_t (v_t - \mu_v), \quad F_t = (I - K_t B) \Sigma_h (I - K_t B)^T + K_t \Sigma_v K_t.$$

Here, $K_t$ is known as Kalman gain matrix. Here is the corresponding MXNet code snippet:

3 The “time series” chapter of the interactive online book “Deep Learning: The Straight Dope”, available at [http://gluon.mxnet.io/index.html](http://gluon.mxnet.io/index.html)
import numpy as np
import mxnet as mx
import mxnet.ndarray as nd
from mxnet.ndarray.linalg import gemm2, potrf, trsm

# ...

if t == 0:
    # At the first time step, use the prior
    mu_h = f_0
    S_hh = F_0
else:
    # Otherwise compute using update eqns.
    mu_h = gemm2(A, f_t)
    S_hh = gemm2(A, gemm2(F_t, A, transpose_b=1)) + S_h

# direct transcription of the update equations above
mu_v = gemm2(B, mu_h)
S_hh_x_B_t = gemm2(S_hh, B, transpose_b=1)
S_vv = gemm2(B, S_hh_x_B_t) + S_v

# use potrf to compute the Cholesky decomposition \( S_{vv} = LL^T \)
S_vv_chol = potrf(S_vv)

# \( K = (S_{hh} B^T) S_{vv}^{-1} = (S_{hh} B^T) L^{-T} L^{-1} \)
K = trsm(S_vv_chol, trsm(S_vv_chol, S_hh_x_B_t, rightside=1, transpose=1),
          rightside=1)

delta = v[t] - mu_v
f_t = mu_h + gemm2(K, delta)

ImKB = eye_h - gemm2(K, B)
F_t = gemm2(ImKB, gemm2(S_hh, ImKB, transpose_b=True))
    + gemm2(K, gemm2(S_v, K, transpose_b=True))

Once more, we compute the Cholesky factor of \( \Sigma_{vv} \) and use backsubstitution instead of computing its inverse, as the latter is less numerically stable.

Note how compared with the traditional parameter learning algorithm, things are much simpler here. Neither do we need expectation maximization, nor the backward pass of Kalman smoothing. This is because the DLDS is taking care of the gradient computations. Once Gaussian LDS are integrated in MXNet, we can fit hybrid models to data. For example, the \( v_t \) could be modeled as sum of a deterministic LSTM and a Gaussian LDS, and parameters of the latter (such as \( A \) or \( \Sigma_v \)) could be parameterized by the LSTM as well. Even time series models with non-Gaussian likelihood, such as \[10\], can be trained in MXNet.

4 Linear Algebra Operators

This section contains the main results of this work: forward and backward expressions for complex linear algebra operators such as Cholesky, LQ and symmetric eigen decomposition, along with details relevant for an efficient implementation. We present final expressions here, their derivations are collected in the Appendix.

\footnote{4 We gloss over some details here, such as the parameterization of the covariance matrices (which have to be kept positive definite).}
4.1 Preliminaries

**Reverse mode differentiation** (RMD) is a calculus for obtaining the gradient \( \partial_x \phi(x) \) of a scalar-valued function \( \phi(x) \). Here, \( x \) is a vector, matrix, or multi-dimensional array. RMD can be seen as generalization of error backpropagation to differentiable directed *computation graphs*. Such bipartite graphs have variable nodes (multi-dimensional arrays) and operator nodes. The predecessor nodes of an operator are its inputs, the successor nodes are its outputs. A computation graph has a single scalar root node (no successors), which we call the *loss* and denote by \( \phi \). The key strength of RMD is *modularity*: a simple graph traversal algorithm can compute the gradients of the loss w.r.t. any other variable node, if only *forward* and *backward* mapping are specified for every operator. In ML applications, certain input nodes (no predecessors) are parameters (weights, biases) to be learned, and this is done by gradient-based minimization of the loss, where RMD is used to compute the gradient.

Suppose we are given an operator \((c, d) = f(a, b)\), with two inputs and two outputs. The forward mapping is just \( f \) itself, with inputs \( a, b \) and outputs \( c, d \). For the backward mapping, we need some notation:

\[
\bar{a} = \partial_a \phi, \quad \bar{c} = \partial_c \phi, \ldots
\]

In its most general UseInOut form, the backward mapping is

\[(\bar{a}, \bar{b}) = f_{\text{back}}(\bar{c}, \bar{d}, a, b, c, d).\]

In other words, the backward mapping computes the input gradients \( \bar{a}, \bar{b} \), given the output gradients \( \bar{c}, \bar{d} \), the inputs \( a, b \), and the outputs \( c, d \). In some cases, the backward mapping requires a subset of these arguments only: \( f_{\text{back}}(\bar{c}, \bar{d}, a, b) \) UseIn or \( f_{\text{back}}(\bar{c}, \bar{d}, c, d) \) UseOut.

RMD proceeds in two passes. In the forward pass, input nodes are bound to data, and all other nodes are computed by forward graph traversal. Note that even though we are formally only interested in the \( \phi \) value, if gradients are required as well, we have to store values of all intermediate nodes. In the backward pass, the gradients \( \bar{a} \) are computed for all variable nodes \( a \) by backward graph traversal.

Highly efficient implementations of RMD, such as MXNet, aim to save memory whenever possible. After all, the main bottleneck of graphics processing units (GPUs) is limited on-board memory. If no gradients are required, there is no need to store intermediate node values, and downstream nodes can be overwritten by upstream ones. Even in forward-backward mode, memory usage can be optimized by rearranging the graph traversal. For our work on operators, it is important that we can signal MXNet that certain outputs can overwrite certain inputs. For example, the code of \( f \) may allow \( c \) to overwrite \( a \), or in \( f_{\text{back}} \), \( \bar{a} \) may overwrite \( \bar{c} \). Another important concept is *in-place computation*. Whenever possible, our forward and backward implementations will employ steps where outputs overwrite inputs not needed anymore, with the goal of using as little temporary memory as possible (most of our operators do not require temporary memory at all).

Finally, note that all our operators support batch operations. Instead of 2D matrices, they also accept 3D tensors. The first dimension is then iterated over. We refer to this variant as *batch mode* below.

**Simple Matrix Functions**

The Hadamard (pointwise) product of two matrices of the same shape is defined as

\[ [A \odot B]_{ij} = a_{ij}b_{ij}. \]

\( \text{sym}(X) \) symmetrizes a square matrix:

\[ \text{sym}(X) = \frac{1}{2} \left( X + X^T \right). \]

\( \text{tril}(X) \) extracts the lower triangle (and diagonal) from a square matrix:

\[ [\text{tril}(X)]_{ij} = x_{ij}1_{(i \geq j)}. \]
copyltu($X$) for a square matrix $X$ generates a symmetric matrix by copying the lower triangle to the upper triangle:

$[\text{copyltu}(X)]_{ij} = \max(i,j)_{\min(i,j)}$.

### BLAS and LAPACK

Our operators are implemented by calling tuned numerical linear algebra code, adhering to the BLAS and LAPACK APIs. For our MXNet implementation, we adopt their naming scheme. For example, the Cholesky decomposition is `dpotrf` in `float64`, `spotrf` in `float32` in LAPACK, while our operator is called `linalg.potrf` (we drop the prefix d or s, since both types are supported via the same operator). Implementations details are given in Section 5. In short, we make use of the existing BLAS dependency for MXNet on CPUs, while using CUBLAS and CUSolver for GPU support.

We only use the simplest flat storage format for matrices in BLAS/LAPACK, avoiding compressed formats for triangular matrices. A lower triangular matrix $L$ has $l_{ij} = 0$ for all $i < j$ (note that the diagonal is non-zero in general). A symmetric matrix $A$ has $a_{ij} = a_{ji}$ for all $i, j$. While BLAS/LAPACK represent symmetric matrices by triangular ones, and only access respective triangles, our MXNet implementation always uses a full square matrix. We note that while it is possible to support compressed matrix formats, and we may do so in the future, such a practice runs against the spirit of DLDS. Once outputs of an operator are not just unconstrained multi-dimensional arrays, it cannot be linked with any other operator.

When using BLAS/LAPACK with MXNet, one additional complication has to be dealt with. BLAS/LAPACK represents matrices in column-major storage:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \Rightarrow [a_{11} \ a_{21} \ a_{12} \ a_{22}] .$$

For whatever reason, MXNet uses row-major storage:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \Rightarrow [a_{11} \ a_{12} \ a_{21} \ a_{22}] .$$

While certain wrappers of BLAS/LAPACK seem to support row-major storage, this often comes at the cost of hidden transpositions and extra memory. Our solution avoids any such conversions. We implement an operator in MXNet by calling respective operators on tranposes internally. For example, we offer the LQ decomposition, but internally call LAPACK code for the QR decomposition (Section 4.3).

### 4.2 Cholesky Decomposition. Related Operators

Derivations of expressions are given in the Appendix. Given a symmetric, positive definite matrix $A$, its Cholesky factor $L$ is lower triangular with positive diagonal, such that $A = LL^T$. forward:

$L = \text{potrf}(A), \ A = LL^T$.

Memory: $L$ can overwrite $A$. No extra memory.

backward: Inputs: $\bar{L}, \ L$ (UseOut).

$$A = \frac{1}{2} L^{-T} \text{copyltu}(L^T \bar{L}) L^{-1}$$

Here, copyltu is defined in Section 4.1. This expression has been given in [8].

Memory: $A$ can overwrite $\bar{L}$. No extra memory.

---

5 We are adding LAPACK wrappers on demand. For CPUs, a BLAS dependency typically includes LAPACK.
6 The same decision has been taken in NumPy long ago.
It is important to note that the computation of $\overline{A}$ is in-place (no extra memory is needed). We start with copying $\overline{L}$ to $\overline{A}$. Both the multiplication with $L^T$ and the backsubstitution operators are in-place BLAS functions.

In order to make `potrf` useful, we implemented a number of additional operators in MXNet. These are listed in the sequel.

**gemm2**

Matrix-matrix multiplication. *forward:*

\[
C = \text{gemm2}(A, B; t_a, t_b, \alpha) = \alpha t_a(A) \cdot t_b(B)
\]

Here, $t(X) = X$ if $t = \text{false}$, $t(X) = X^T$ if $t = \text{true}$.

No extra memory required.

*backward: Inputs: $\overline{C}$, $A$, $B$ (UseIn).*

\[
\overline{A} = \left\{ \begin{array}{c}
gemm2(\overline{C}, B; t_a, t_b, \alpha), & t_a = \text{false} \\
gemm2(B, \overline{C}; t_b, t_a, \alpha), & t_a = \text{true}
\end{array} \right. \quad \overline{B} = \left\{ \begin{array}{c}
gemm2(A, \overline{C}; t_a, t_b, \alpha), & t_b = \text{false} \\
gemm2(\overline{C}, A; t_b, t_a, \alpha), & t_b = \text{true}
\end{array} \right.
\]

Memory: $B$ can overwrite $A$, given that $\overline{A}$ is computed before $\overline{B}$. No extra memory required.

Note that the general matrix-matrix multiplication does not allow for in-place computation. It is maybe surprising that such an operator has to be added to MXNet, given that most neural networks contain densely connected layers. The reason is that other MXNet operators do not consistently support `float64`, and may also be unwieldy to use.

**trmm**

Multiplication with lower triangular matrix (in-place). There are four different cases. *forward:*

\[
B = \text{trmm}(L, A; t_l, \text{rightside} = \text{false}) = t_l(L)A,
\]
\[
B = \text{trmm}(L, A; t_l, \text{rightside} = \text{true}) = A t_l(L)
\]

$L$ is lower triangular. $t(X) = X$ if $t = \text{false}$, $t(X) = X^T$ if $t = \text{true}$.

Memory: $B$ can overwrite $A$. No extra memory.

*backward: Inputs: $B$, $L$, $A$ (UseIn).*

\[
B = LA \Rightarrow \overline{A} = L^T \overline{B}, \quad \overline{L} = \text{tril} \left( \overline{B}A^T \right),
\]
\[
B = L^T A \Rightarrow \overline{A} = LB, \quad \overline{L} = \text{tril} \left( AB^T \right),
\]
\[
B = AL \Rightarrow \overline{A} = BL^T, \quad \overline{L} = \text{tril} \left( A^T B \right),
\]
\[
B = AL^T \Rightarrow \overline{A} = BL, \quad \overline{L} = \text{tril} \left( B^T A \right)
\]

Memory: $\overline{A}$ can overwrite $\overline{B}$, given that $\overline{L}$ is computed first. No extra memory.

Note that not only is `trsm` faster than `gemm2`, it is also in-place, so that $B$ can overwrite $A$.

**trsm**

Backsubstitution with lower triangular matrix (in-place). There are four different cases. *forward:*

\[
B = \text{trsm}(L, A; t_l, \text{rightside} = \text{false}) = t_l(L)^{-1} A,
\]
\[
B = \text{trsm}(L, A; t_l, \text{rightside} = \text{true}) = A t_l(L)^{-1}
\]
$L$ is lower triangular. $t(X) = X$ if $t =$ false, $t(X) = X^T$ if $t =$ true.

Memory: $B$ can overwrite $A$. No extra memory.

*backward:* Inputs: $\bar{B}$, $L$, $A$, $B$ (UseInOut).

\[
B = L^{-1}A \Rightarrow \bar{A} = L^{-T}\bar{B}, \quad \bar{L} = -\text{tril} \left( \bar{A}B^T \right),
\]
\[
B = L^{-T}A \Rightarrow \bar{A} = L^{-1}\bar{B}, \quad \bar{L} = -\text{tril} \left( B\bar{A}^T \right),
\]
\[
B = AL^{-1} \Rightarrow \bar{A} = \bar{B}L^{-T}, \quad \bar{L} = -\text{tril} \left( B^T\bar{A} \right),
\]
\[
B = AL^{-T} \Rightarrow \bar{A} = \bar{B}L^{-1}, \quad \bar{L} = -\text{tril} \left( \bar{A}^TB \right).
\]

Memory: $\bar{A}$ can overwrite $B$ or $A$. $\bar{L}$ can overwrite $L$. Here, $\bar{A}$ has to be computed first. No extra memory.

**syrk**

Multiplication of matrix with own transpose. *forward:*

\[
B = \text{syrk}(A; \tau_a, \alpha) = \alpha\tau_a(A) \cdot \tau_a(A).
\]

Here, $t(X) = X$ if $t =$ false, $t(X) = X^T$ if $t =$ true.
No extra memory required.

*backward:* Inputs: $\bar{B}$, $A$ (UseIn). Note that $\bar{B}$ need not be symmetric.

\[
B = \alpha AA^T \Rightarrow \bar{A} = 2\alpha(\text{sym} \bar{B})A,
\]
\[
B = \alpha A^TA \Rightarrow \bar{A} = 2\alpha A(\text{sym} \bar{B})
\]

No extra memory required.

**potri**

Computation of inverse $A^{-1}$, given the Cholesky factor $L$ of $A$, where $A$ is symmetric, positive definite. $L$ lower triangular with positive diagonal. *forward:*

\[
B = \text{potri}(L) = A^{-1}, \quad A = LL^T.
\]

Memory: $B$ can overwrite $L$. No extra memory required.

*backward:* Inputs: $\bar{B}$, $L$, $B$ (UseInOut). Note that $\bar{B}$ need not be symmetric:

\[
\bar{L} = -2\text{tril} \left( B \text{sym}(\bar{B})L^{-T} \right).
\]

No extra memory required.

This operator is needed only in special circumstances. For example, some algorithms require the diagonal of the inverse of $A$. However, most expressions in ML algorithms can be computed with the Cholesky factor alone, together with $\text{trmm}$ and $\text{trsm}$. For example, the $\phi$ expression in Section 3.1 contains $A^{-1}$, but the code does not use $\text{potri}$. As a general rule, explicit computation of the inverse $A^{-1}$ should be avoided whenever possible: inversion is subject to a lot more numerical error than Cholesky factorization alone.

### 4.3 LQ Decomposition

Derivations of expressions are given in the Appendix. Suppose that $A \in \mathbb{R}^{m \times n}$, where $m \leq n$. The LQ decomposition is

\[
A = LQ, \quad QQ^T = I_m, \quad l_{ij} = 0 \ (i < j).
\]
Here, \( Q \in \mathbb{R}^{m \times n} \) is row-orthonormal, and \( L \in \mathbb{R}^{m \times m} \) is lower triangular with non-zero diagonal. We require that \( A \) has full rank: \( \text{rk} A = m \).

**forward:** \((Q, L) = \text{gelqf}(A), \quad A = LQ, \quad QQ^T = I_m.\)

Memory: \( Q \) can overwrite \( A \). Additional workspace memory is required.

**backward:** Inputs: \( \bar{Q}, \bar{L}, Q, L \) (UseOut). Note that \( \bar{L} \) need not be lower triangular:

\[
\bar{A} = L^{-T}(Q + \text{copyltu}(M)Q), \quad M = L^T\bar{L} - \bar{QQ}^T.
\]

Here, copyltu is defined in Section 4.1. This expression is novel to the best of our knowledge.

Memory: \( \bar{A} \) can overwrite \( \bar{Q} \). One temporary \( \mathbb{R}^{n \times m} \) matrix is required.

### Implementation Details

LAPACK code for the LQ factorization is more complicated than for Cholesky. First, we have to call two LAPACK routines: \text{gelqf}, followed by \text{orglq}. The first returns \( Q \) in an internal storage format, which is converted to matrix form by the second. Second, both routines require working space, the amount of which depends on \( n, m \) and internal parameters. The amount of working space has to be requested by a workspace query. Our implementation calls these queries and allocates workspace space accordingly. In batch mode, workspace is allocated once only, then used for all items of a batch.

The column versus row-major issue was noted in Section 4.1. This means that internally, we compute the QR decomposition of \( A^T \), calling LAPACK \text{geqrf} and \text{orgqr}. For ML applications, we can always use the LQ factorization in place of the QR factorization. Given that LAPACK offers both LQ and QR factorization, why do we not offer both as well? It turns out that the current version of CUSolver only contains the QR factorization (in column-major).

### 4.4 Symmetric Eigendecomposition

Derivations of expressions are given in the Appendix. Given a symmetric matrix \( A \in \mathbb{R}^{n \times n} \), its eigendecomposition is

\[
A = U^T(\text{diag} \lambda)U, \quad U^TU = I.
\]

Here, \( U \) is orthonormal, and the eigenvalues are ascending: \( \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \). The rows of \( U \) are the eigenvectors corresponding to eigenvalues. In order for derivatives to be defined, all eigenvalues of \( A \) must be distinct. Our implementation still works if \( \lambda \) has very small or zero eigengaps, but in this case, **backward** is approximate. Note that if the entries of \( A \) are drawn i.i.d. at random (subject to being symmetric), the eigenvalues are distinct with probability one. However, the user has to be careful not to apply \text{syevd} to matrices such as \( I + XX^T \), which have multiple eigenvalues by design. **forward:**

\[
(U, \lambda) = \text{syevd}(A), \quad A = U^T(\text{diag} \lambda)U, \quad U^TU = I.
\]

Memory: \( U \) can overwrite \( A \). Additional workspace memory is required.

**backward:** Inputs: \( \bar{U}, \bar{\lambda}, U, \lambda \) (UseOut):

\[
\bar{A} = U^T \left( \text{sym}(U^TU \circ F) + \bar{A} \right)U, \quad F_{ij} = \frac{1_{\{i\neq j\}}}{h(\lambda_i - \lambda_j)}, \quad h(t) = \max(|t|, \varepsilon) \text{sgn}(t),
\]

and \( \varepsilon > 0 \) is a small scalar. Note that using \( h(\cdot) \) amounts to an approximation. The correct expression has \( h(t) = t \), resulting in numerical errors for vanishing eigengaps. This expression is given in \([5]\).

Memory: \( \bar{A} \) can overwrite \( \bar{U} \). One temporary matrix of the shape of \( \bar{A} \) is needed.

---

\(^{7}\) The operator does not have derivatives at rank-deficient \( A \).
If \( Y = \text{sym}(X \circ F) \), then \( y_{ii} = 0 \), and for \( i > j \):

\[
y_{ij} = \frac{x_{ij} - x_{ji}}{2h(\lambda_i - \lambda_j)} = \frac{x_{ij} - x_{ji}}{2 \max(\lambda_i - \lambda_j, \varepsilon)}, \quad \text{since} \ \lambda_i \geq \lambda_j.
\]

One additional issue has to be dealt with: the signs of eigenvectors are not well defined. In other words, if \( U \) collects eigenvectors of \( A \), so does \((\text{diag} \sigma) \bar{U}\), where \( \sigma_i \in \{\pm 1\} \). The backward expression is invariant to sign changes only if \( \bar{U} \) is replaced by \( (\text{diag} \sigma) \bar{U} \) as well. Denote the \( i \)-th row of \( U \) by \( u_i \). We need a deterministic rule to decide upon the sign of each \( u_i \). Any rule which splits the unit sphere in half will do. Our implementation determines \( k_i = \arg\max_k |u_{ik}| \). If \( u_{ik} < 0 \), then \( u_i \) is replaced by \(-u_i\). In case of a tie, the sign is determined by the smaller index \( k_i \). Note that any such rule does give rise to further (isolated) inputs \( A \) at which derivatives are not well defined.

**Implementation Details**

The standard LAPACK routine for symmetric eigendecomposition is \texttt{syevd}. Note that there is a variant \texttt{syevr}, which is reported to be faster and to require less memory. On the flip side, calling \texttt{syevr} is slightly more involved, and \( U \) cannot overwrite \( A \). Also, this routine is not currently implemented in CUSolver. Our current implementation uses \texttt{syevd} on both CPU and GPU, leaving the support of \texttt{syevr} on the CPU for future work.

The column versus row-major issue was noted in Section 4.1. This means that internally, we compute the factorization \( A = U (\text{diag} \lambda) U^T \), where eigenvectors are columns of \( U \).

5. **Implementation in MXNet**

In this section, we provide details on our implementation of differentiable linear algebra operators in the MXNet\(^8\) DLDS. Different to TensorFlow, which depends on Eigen (see Section 2.1), MXNet did not support linear algebra expressions beyond matrix-matrix multiplication before our extension. We decided to implement the new operators directly in the core C++ kernel of MXNet, instead of going for a Python based extension, as is the case for TensorFlow\(^9\). Doing so enabled us to

- ensure maximum performance and efficiency of the operator implementations
- minimize the memory footprint of the operators, by exploiting all opportunities for in-place computations and memory re-usage (as the C++ core of MXNet allows fine-grained control over memory management)
- leverage the MXNet intrinsic mechanisms that allow contributors to write a single C++ implementation, from which language bindings for all supported languages (Python, Scala, Julia, Perl, R) are automatically generated, both for imperative and declarative programming models

The implementation is broken up into several MXNet-internal layers of abstraction. The goal was to provide an infrastructure for linear algebra operations within MXNet that is efficient and extendable. We anticipate that there will be demand for adding further functionality in the future, and want to lay out a specific software pattern for future contributors. This makes it easier to add new operators for linear algebra, and at the same time helps maintaining a consistent code structure.

For CPU support, we integrated the LAPACK library into MXNet in addition to the already imported BLAS library. Integration is done by interfacing directly to the Fortran code. We decided against using

\(^8\) [https://github.com/apache/incubator-mxnet](https://github.com/apache/incubator-mxnet)

\(^9\) This may be due to the fact that open source extensions to TensorFlow are limited to its Python API, while MXNet invites open source contributions to its core just as well.
existing C wrappers of LAPACK, such as `lapacke`. These are not consistently available across all MXNet-supported platforms, and they tend to be implemented inefficiently, relying on unnecessary transpositions and temporary copies in order to bridge between row-major and column-major storage. In contrast, our wrappers are consistently in-place. They may modify arguments (such as flipping flags for upper or lower triangle, or transposition), the input operand order, and sometimes even the type of the requested computation (such as calling the LAPACK QR factorization on the transpose matrix, see Section 4.3). As a result, the desired computation in row-major layout (MXNet) is translated into an equivalent computation based on column-major layout (LAPACK, BLAS) without any performance or memory penalty.

We decided against wrapping the entire BLAS and LAPACK APIs in one shot, but only imported functions which were required in the scope of this project. We feel it is best to integrate functionality on demand, each time carefully reducing computation overhead, rather than mechanically integrating the full library.

For GPU support, we integrated the cuSOLVER library (https://developer.nvidia.com/cusolver) into MXNet, in addition to the already imported cuBLAS library (https://developer.nvidia.com/cublas). cuSOLVER implements a subset of the LAPACK API and is specifically tuned for NVidia GPUs. The subset covers all functions needed for our operators, except `potri` (inverse from Cholesky factor). We implemented `potri` for GPUs by two calls to `trsm`. Since cuSOLVER assumes column-major storage, we applied the techniques described above to map to the row-major layout required for MXNet.

The second abstraction layer implements a unified tensor-based C++ interface for BLAS/LAPACK functions. It provides overloaded functions that execute the same linear algebra operations on CPU or GPU and supports processing individual matrices as well as batch mode operations that involve multiple matrices having the same dimensions. This layer hides all aspects of matrix memory layout, differences in function signatures between CPU and GPU versions, and details of parallel processing from the caller. It also hides the fact that `float32` and `float64` BLAS/LAPACK functions have different names. The currently supported operators are detailed in Section 4.

MXNet internally follows a program pattern, where input and output tensors of an operator are located either on the CPU or one of multiple GPUs. The execution context of an operation can therefore be deduced from its arguments, it does not have to be specified. This convenient pattern allows to write most code in a generic fashion, independent of the execution device.

The third abstraction layer is built entirely on top of the second one, and is therefore agnostic to CPU or GPU usage, as well as data type. It provides C++ methods for doing efficient forward and backward computations of the linear algebra operators. The forward computation is usually a direct call to the second layer methods, while the backward computation comprises of a series of basic linear algebra operations. As noted in Section 4, most backward computations are entirely in-place. This is possible because the BLAS/LAPACK API supports in-place whenever possible, and so does our second layer.

Based on the third abstraction layer, high level operators have been added to MXNet that are accessible to the user in a multitude of different languages. Creating such operators involves packaging of the linear algebra methods into data structures that are understood by core MXNet components, such as the scheduler and the memory manager. MXNet provides a convenient registry mechanism for accomplishing this. It only requires to register C++ functions for the forward and backward pass that should be executed whenever the operator is invoked as part of a user program. Alongside with the entry points to these functions, additional attributes can be supplied that control memory allocation and memory re-usage, parameter passing, type checking and even documentation. Leveraging the registry and using generic templated wrappers around the various linear algebra methods, all linear algebra operators visible to the user are realized in a concise and unified way.

6 Discussion

We have shown how to introduce advanced linear algebra routines, such as Cholesky factorization, back-substitution, LQ factorization, and symmetric eigen decomposition, as differentiable operators into a deep

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10 As noted in Section 4, we sometimes require workspace queries and allocation as well.
learning development system (DLDS). Implemented in a time and memory efficient manner, they open the
door to realizing a host of “pre-deep” machine learning models within a DLDS, and enable combinations
of Gaussian processes, Bayesian linear models, or linear dynamical systems with deep multi-layer maps. We
provide a range of machine learning examples, complete notebooks for which are available for download.

All operators mentioned here are implemented in MXNet (https://github.com/apache/incubator-mxnet).
In contrast to similar operators in TensorFlow and Theano, our implementation is tuned for maximum
memory efficiency. We call highly optimized BLAS and LAPACK library functions directly on the C++
level. In particular, we take care to use the minimum required amount of temporary storage. Most of our
operators are implemented in-place, meaning that no additional memory is needed beyond inputs and
outputs. If memory-intensive machine learning or scientific computing methods (such as Gaussian processes,
least squares estimation, Kalman smoothing, or principal components analysis) are to be powered by
easy-to-use DLDS, it will be essential to implement key linear algebra operators with the same level of care
that is applied to convolution or LSTM layers today.

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in the “Deep Learning: The Straight Dope” online book, containing a full-fledged Kalman filtering imple-
mentation, using our novel operators. Moreover, we would like to thank the core developers and the open
source community around MXNet for much help and support.

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In this section, we collect derivations for backward expressions of supported operators. Note that some operators are not covered, in case the respective derivations are obvious, given the ones reported here.

**potrf**

This derivation is given in [8]. Recall that \( A = LL^T \), where \( A \) is symmetric, \( L \) is lower triangular. We first determine \( dA \) in terms of \( dL \) and inputs. Differentiate the defining equation, and apply \( L^{-1}(dL) \):

\[
L^{-1}(dA)L^{-T} = 2 \text{sym}(L^{-1}(dL)),
\]

Importantly, \( L^{-1}(dL) \) is lower-triangular, so we really only have to equate the lower triangle on both sides (taking care of the diagonal). Define the lower triangular “masking matrix” \( E \in \mathbb{R}^{n \times n} \) by

\[
e_{ij} = \begin{cases} 
0 & | i < j \\
1 & | i = j \\
2 & | i > j 
\end{cases}
\]

Then we have:

\[
dL = \frac{1}{2} L \left( L^{-1}(dA)L^{-T} \circ E \right).
\]

For the backward expression:

\[
d\phi = \text{tr} \bar{L}^T(dL) = \frac{1}{2} \text{tr} \bar{L}^T L(L^{-1}(dA)L^{-T} \circ E) = \frac{1}{2} \text{tr}(L^T \bar{L} \circ E)^T L^{-1}(dA)L^{-T}.
\]

We used that \( \text{tr} X^T(Y \circ E) = \text{tr}(X \circ E)^T Y \). Note that \( \bar{A} \) must be symmetric. Therefore:

\[
\bar{A} = \frac{1}{2} L^{-T} \text{sym}(L^T \bar{L} \circ E)L^{-1}.
\]

Note that \( \text{sym}(X \circ E) = \text{copyltu}(X) \), so that

\[
\bar{A} = \frac{1}{2} L^{-T} \text{copyltu}(L^T \bar{L})L^{-1}.
\]

**gelqf**

To the best of our knowledge, this derivation is novel. Recall that \( A = LQ \), where \( A, Q \in \mathbb{R}^{m \times n} \), \( L \in \mathbb{R}^{m \times m} \). Also, \( QQ^T = I_m \), and \( L \) is lower triangular with nonnegative diagonal. First:

\[
dA = (dL)Q + L(dQ) \Rightarrow dQ = L^{-1}(dA - (dL)Q).
\]

Differentiating \( QQ^T = I_m \), we note that \( (dQ)Q^T \) is skew-symmetric (meaning that \( X^T = -X \)). Multiplying the above equation by \( Q^T \) on the right:

\[
(dQ)Q^T = C - L^{-1}(dL), \quad C := L^{-1}(dA)Q^T.
\]
Using the skew-symmetry:
\[
C - L^{-1}(dL) = (L^{-1}(dL))^T - C^T \quad \Rightarrow \quad \text{sym}(C) = \text{sym}(L^{-1}(dL)).
\]
Since \(L^{-1}(dL)\) is lower triangular, we use the same argumentation as for \texttt{potrf} above:
\[
dL = L (\text{sym}(C) \circ E).
\]
Plugging these into \(d\phi\), we obtain
\[
d\phi = \text{tr} \left( L^{-T} \tilde{Q} \right)^T (dA) + \text{tr} \left( \bar{L} - L^{-T} \tilde{Q} Q^T \right)^T (dL).
\]
Plugging \(dL\) into the second term:
\[
\text{tr}(. . .)^T (dL) = \text{tr} M^T (\text{sym}(C) \circ E) = \text{tr} \text{sym}(M \circ E) C, \quad M \coloneqq L^T \bar{L} - QQ^T.
\]
Plugging in \(C\), some further algebra gives
\[
\tilde{A} = L^{-T} (\tilde{Q} + \text{sym}(M \circ E) \tilde{Q}) = L^{-T} (\tilde{Q} + \text{copyltu}(M) \tilde{Q}).
\]

\textbf{syevd}

This derivation is given in \[5\]. Let \(A \in \mathbb{R}^{n \times n}\) be symmetric. Recall that \(U A = \Lambda U\), where \(\Lambda = \text{diag} \Lambda\), and \(UU^T = I\). Differentiating the equation and right-multiplication with \(U^T\) gives:
\[
U(dA)U^T + (dU)U^T \Lambda = \Lambda(dU)U^T + d\Lambda,
\]
where we used that \(AU^T = U^T \Lambda\). Denote \(M \coloneqq U(dA)U^T, \quad S \coloneqq (dU)U^T\).

Differentiating \(UU^T = I\), we see that \(S\) is skew-symmetric, and in particular \(\text{diag}(S) = 0\). The equation becomes
\[
M + S \Lambda = \Lambda S + d\Lambda.
\]
Now, \(\text{diag}(A S) = \lambda \circ \text{diag}(S) = 0\), so that
\[
d\lambda = \text{diag}(M)
\]
Denote \(\tilde{M} := M - (M \circ I)\), whose diagonal is zero. Now:
\[
A S - S \Lambda = [s_{ij}(\lambda_i - \lambda_j)]_{i,j} = \tilde{M}.
\]
Therefore: \(s_{ij} = \tilde{m}_{ij}/(\lambda_i - \lambda_j)\) for \(i \neq j\), and \(s_{ii} = 0\). Define the matrix \(F \in \mathbb{R}^{n \times n}\) as
\[
F_{ij} = \frac{I_{i \neq j}}{\lambda_i - \lambda_j},
\]
where the indicator has preference, so that \(F_{ii} = 0\). Then: \(S = \tilde{M} \circ F\), therefore
\[
dU = (\tilde{M} \circ F)U = (M \circ F)U,
\]
since \(\text{diag}(F) = 0\). Then:
\[
d\phi = \text{tr} \bar{U}^T (dU) + \bar{\Lambda}^T (d\lambda) = \text{tr}UU^T (M \circ F) + \text{tr} \bar{\Lambda} M = \text{tr} \left( \bar{U}U^T \circ F + \bar{\Lambda} \right)^T M.
\]
Plugging in \(M\), and noting that it is symmetric, some algebra gives:
\[
\bar{A} = U^T \left( \text{sym}(\bar{U}U^T \circ F) + \bar{\Lambda} \right) U.
\]
When working with \(F\), we need to guard against division by zero. Therefore, we use a slight modification:
\[
F_{ij} = \frac{I_{i \neq j}}{h(\lambda_i - \lambda_j)} = h(t) = \max(|t|, \varepsilon) \text{sgn}(t),
\]
and \(\varepsilon > 0\) is a small scalar.
trsm
We work out backward for $B = L^{-1}A$, the other cases are similar.

$$dB = L^{-1}(dA) - L^{-1}(dL)L^{-1}A$$

From this, we obtain

$$dφ = tr \bar{B}^T(dB) = tr \left( (L^{-T}\bar{B})^T(dA) + tr \left( -L^{-T}\bar{B}A^T L^{-T} \right)^T (dL) \right).$$

Therefore:

$$\bar{A} = L^{-T} \bar{B}, \quad \bar{L} = - tril \left( AA^T L^{-T} \right) = - tril \left( AB^T \right).$$

Here, tril(·) extracts the lower triangle.
Note that $A$ is not needed (but $L$ is). We have to compute $\bar{A}$ first. It can overwrite $\bar{B}$ or $A$. Also, $\bar{L}$ can overwrite $L$.

trmm
We work out backward for $B = LA$, the other cases are similar.

$$dB = (dL)A + L(dA)$$

gives

$$\bar{A} = L^T \bar{B}, \quad \bar{L} = tril \left( BA^T \right).$$

This can be done in-place. We compute $\bar{L}$ first, in which case $\bar{A}$ can overwrite $\bar{B}$.

potri
The operator is $B = A^{-1} = dpotri(L)$. Note that $B$ is symmetric. We have

$$dB = -B(dA)B = -2B \text{sym} \left( (dL)L^T \right) B = -2 \text{sym} \left( B(dL)L^{-1} \right),$$

using $B = L^{-T}L^{-1}$. We must not assume that $B$ is symmetric: $tr B^T \text{sym}(X) = tr \text{sym}(B)X$. Therefore:

$$dφ = -2 tr \text{sym}(\bar{B})B(dL)L^{-1}.$$

This gives

$$\bar{L} = -2 \text{tril} \left( B \text{sym}(\bar{B})L^{-T} \right).$$

This can be done in-place. Here, outputs cannot overwrite inputs. In fact, our implementation uses

$$2B \text{sym}(\bar{B}) = B\bar{B} + B\bar{B}^T,$$

even if this is slightly wasteful, in order to avoid having to allocate temporary memory for $\text{sym}(\bar{B})$. 