THESIS DEFENSE

FInC Flow: Fast and Invertible k × k Convolutions for Normalizing Flows

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Outline

- Prerequisites Generative Al
- Normalizing Flows
- Convolution A Linear Transformation
- Inverse of convolution
- Inverse Techniques
- FInC Flow Our Work
- GPU implementation



 Generative AI refers to a class of artificial intelligence algorithms that have the capability to generate new content, such as text, images, or other forms of data, based on patterns and information present in the training data

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- Text: GPT-3, Chat-GPT, PaLM, Llama etc.
- Images: GAN, StyleGAN, DeepCream
- Art: DALL-E, Aiva
- Audio: GANs, Normalizing Flows, VAE models

Involves around 4 types of generative models:

- 1. GAN(Generative Adversarial Networks): The generator creates synthetic data, while the discriminator evaluates whether the generated data is real or fake.
- 2. VAE(Variational Auto Encoders): Consists of an Encoder which compresses the data and a Decoder which tries to get the original data from a compressed encoded data
- 3. Normalizing Flows: Generates data by simply transforming a Normal Distribution by a series of invertible and differentiable functions
- 4. Diffusion Models: These models transform a simple and known distribution (e.g., Gaussian noise) into a complex and high-dimensional distribution that matches the characteristics of the target data.

Why Normalizing Flows

- 1. Use of bijective and differentiable allows models for easy generation and manipulation of data
- 2. Exact Likelihood: Unlike all the other models, we can actually compute the probability distribution of the data
- 3. Flexible and Explicit Density Modeling
- 4. Versatile data generation

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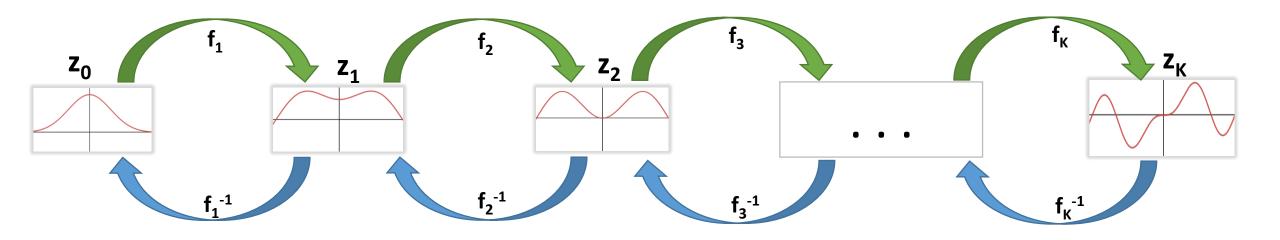
But the generation of samples can be extremely slow

Our Contributions

We develop a system/model which

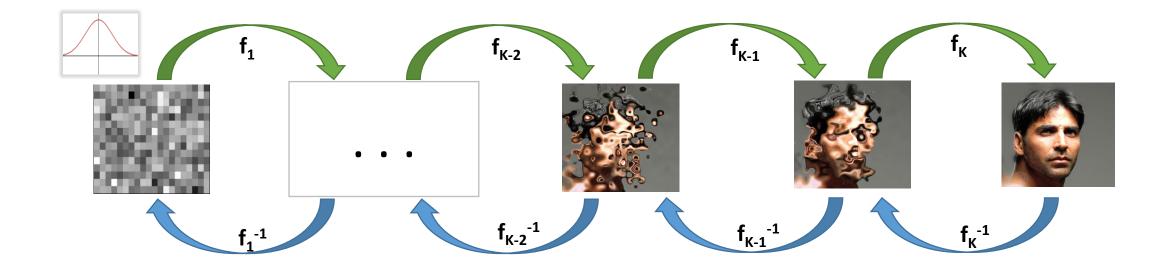
- 1. has a fast parallel inversion algorithm with running time O(nk²) (n is height and width of the input image and k is kernel size)
- 2. masks the minimal amount of learnable parameters in a layer
- 3. gives better sampling time comparable to other k × k convolution-based models on real-world benchmarks.

Normalizing Flows

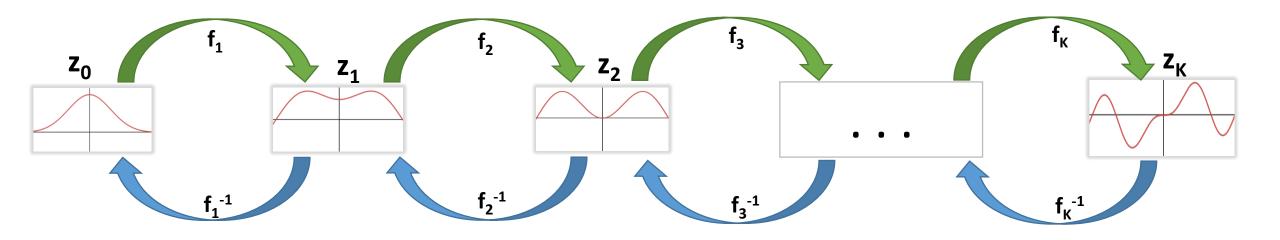


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Normalizing Flows



Normalizing Flows



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Let zo E IR be a multivariate R.V. with density Po(zo)

Let $z_0 \in \mathbb{R}^p$ be a multivariate R.V. with density $P_0(z_0)$ For i = 1, 2, ..., K, let $z_i = f_i(z_{i-1})$ be a sequence of transformations of z_0

Let
$$z_0 \in \mathbb{R}^p$$
 be a multivariate R.V. with density $P_0(z_0 = 1, 2, ..., K$, let $z_i = f_i(z_{i-1})$ be a sequence of transformations of z_0
Then log likelyhood of z_K is $\log P_K(z_K) = \log P_0(z_0) - \sum_{i=1}^{K} \log \left| \det \frac{\partial f_i(z_{i-1})}{\partial z_{i-1}} \right|$

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 $\log P_k(z_k) = \log P_o(z_0) - \sum_{i=1}^k \log \left| \det \frac{\partial f_i(z_{i-1})}{\partial z_{i-1}} \right|$

Derivation:

$$z_{1} = f_{1}(z_{0}) ; z_{0} = f_{1}^{-1}(z_{1})$$

$$P_{1}(z_{1}) = P_{0}(z_{0}) | det \frac{\partial f_{1}^{-1}(z_{1})}{\partial z_{1}} |$$

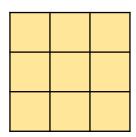
$$P_{1}(z_{1}) = P_{0}(z_{0}) | det \left(\frac{\partial f_{1}(z_{0})}{\partial z_{0}}\right)^{-1} |$$
By the identity, $det(A^{-1}) = (det A)^{-1}$

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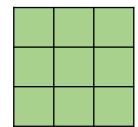
 $P_{1}(z_{1}) = P_{0}(z_{0}) \left| \det \frac{\partial f_{1}(z_{0})}{\partial z_{0}} \right|^{-1}$
 $\log P_{1}(z_{1}) = \log P_{0}(z_{0}) - \log \left| \det \frac{\partial f_{1}(z_{0})}{\partial z_{0}} \right|$
The above equation applies to any z_{1}, z_{i-1}
 $\log P_{K}(z_{K}) = \log P_{K-1}(z_{K-1}) - \log \left| \det \frac{\partial f_{K}(z_{K-1})}{\partial z_{K-1}} \right|$
But $\log P_{K-1}(z_{K-1}) = \log P_{K-2}(z_{K-2}) - \log \left| \det \frac{\partial f_{K-1}(z_{K-2})}{\partial z_{K-2}} \right|$
 \vdots
 $\log P_{K}(z_{K}) = \log P_{0}(z_{0}) - \sum_{i=1}^{K} \log \left| \det \frac{\partial f_{i}(z_{i-1})}{\partial z_{i-1}} \right|$

Convolution

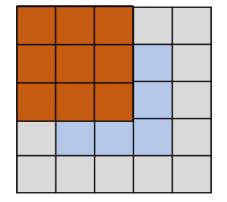


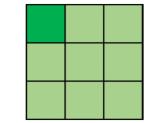
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Convolution





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Convolution – Padding, Stride, Step

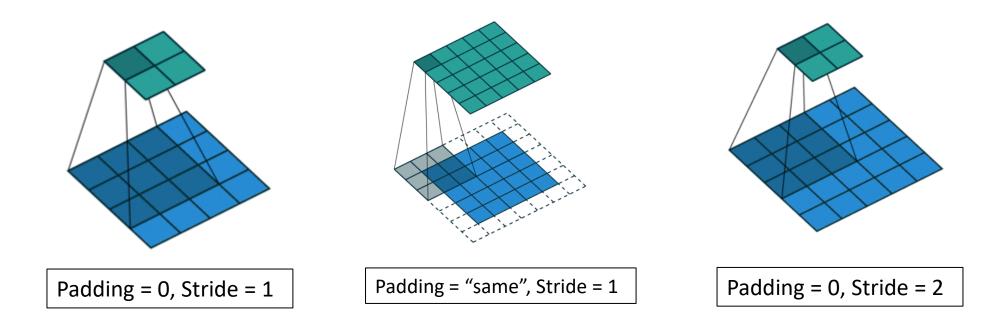


Image Credits: https://hannibunny.github.io/mlbook/neuralnetworks/convolutionDemos.html

- n Height and Width of an image
- H Height of an image
- W Width of an image
- k Height and Width of a convolution filter (kernel)
- k x k Size of a kernel
- C Number of channels
- * Convolution operator

Convolution – A Linear Transformation

- At each step of the convolution, k x k multiplications occur
- In other words, every value in the output can be thought of as a linear function of kernel weights and subset of input (that is, input values in the corresponding window)
- In fact, we can say input is being linearly transformed by a matrix (M) referred to as Convolution Matrix

Convolution – A Linear Transformation

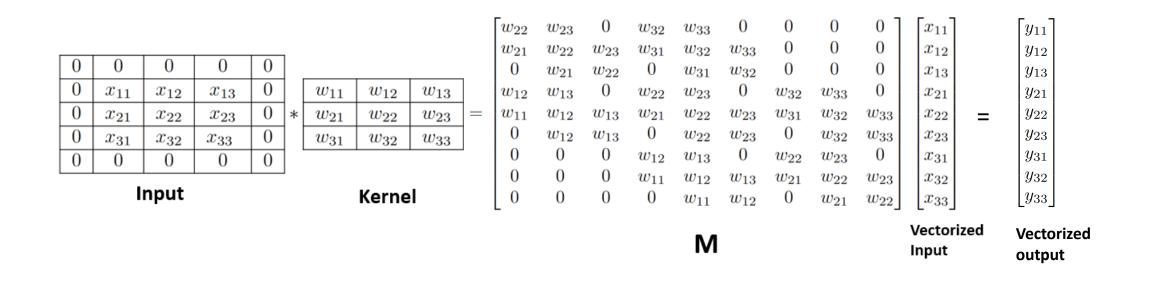


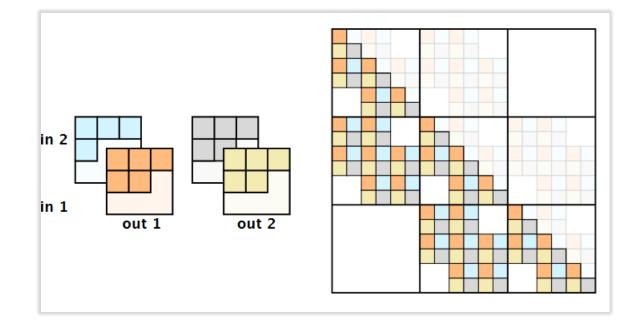
Fig. General Convolution – A linear transformation. **M**, the Convolution Matrix

Inverse Techniques

Emerging Flows

- Leverages the fact that convolution is associative
- Two Auto regressive Convolutions are chained
- Each of the Auto regressive Convolution is chosen so that **M** is triangular
- Inverse Time is O(n²k²)

 $K_{2}^{*}(K_{1}^{*}X) = (K_{2}^{*}K_{1}^{*}) * X$

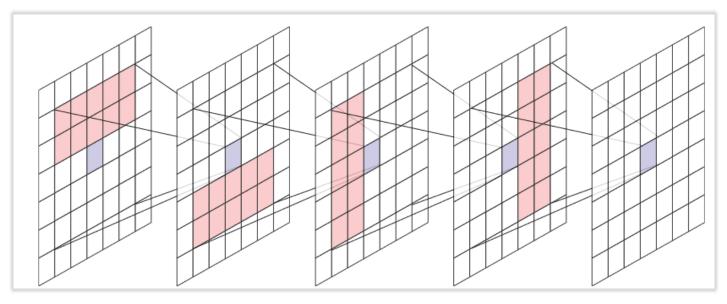


Credits: Hoogeboom, E., Van Den Berg, R., and Welling, M. (2019). Emerging convolutions for generative normalizing flows. In International Conference on Machine Learning, pages 2771–2780. PMLR.

Convolution Techniques

MACOW: Masked Convolutional Flow

- Leverages the fact that convolution is associative
- Four Masked Convolutions are chained
- Inverse Time is O(nk²)



Credits: Ma, X., Kong, X., Zhang, S., and Hovy, E. (2019). Macow: Masked convolutional generative flow. Advances in Neural Information Processing Systems, 32.

Inverse Techniques

CInC Flow

- Padding the input is done so that the resulting M is triangular
- Very minimal amount of masking required
- Requires only 1 filter per convolution
- Inverse Time is O(n²k²)

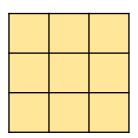
Credits: Nagar, S., Dufraisse, M., and Varma, G. (2021). Clnc flow: Characterizable invertible 3 x 3 convolution. In The 4th Workshop on Tractable Probabilistic Modeling.

Inverse Techniques

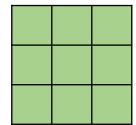
- We observe that techniques mask much of the kernel values and thus resulting in needing more kernels
- We observe that the inverse time is O(n²k²)
- Can we do better?

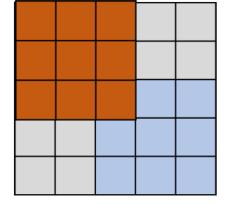
Method	# of ops	# params / CNN layer	Complexity of Jacobian	Inverse
FInC Flow Woodbury McCow	$(2n-1)k^2$ cn^2 $4nk^2$	k^2	$1 \\ O(d^2(c+n) + d^3) \\ O(n^3)$	exact exact
MaCow Emerging CInC Flow	$ \frac{4nk^2}{2n^2k^2} n^2k^2 $	$k(\lceil \frac{k}{2} \rceil - 1) k(\lceil \frac{k}{2} \rceil - 1) k^2 - 1$	$O(n^2)$ O(n) 1	exact exact exact
MintNet SNF	3n k^2	$\frac{\frac{k^2}{3}}{k^2}$	O(<i>n</i>) approx	approx approx

n x *n* – Size of the image; *c* – Number of Channels; *k* x *k* – Filter Size; *d* – Intermediate Latent Dimension Space

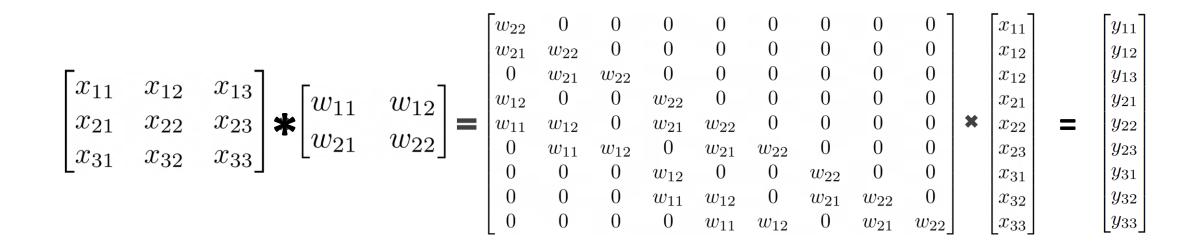


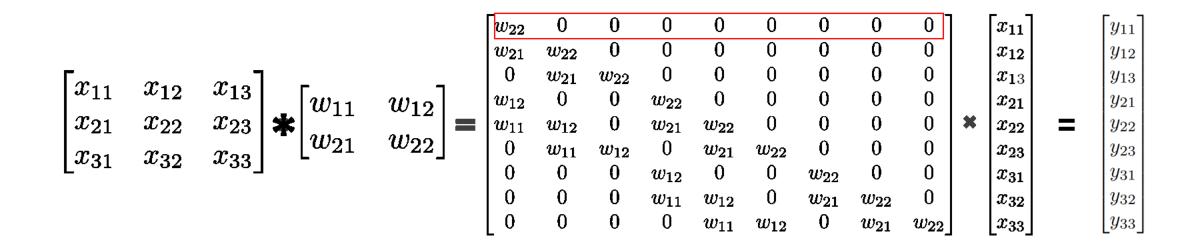


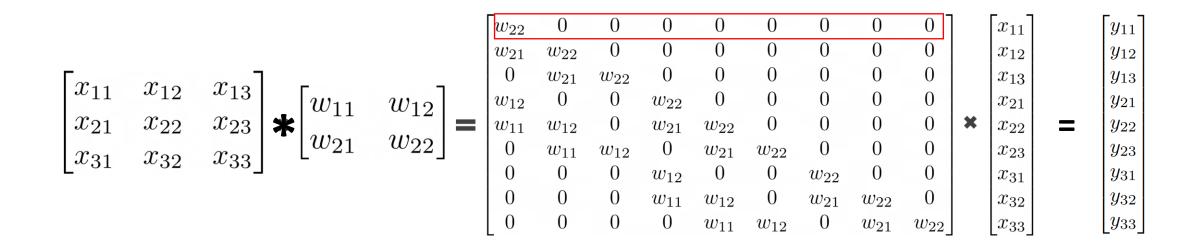




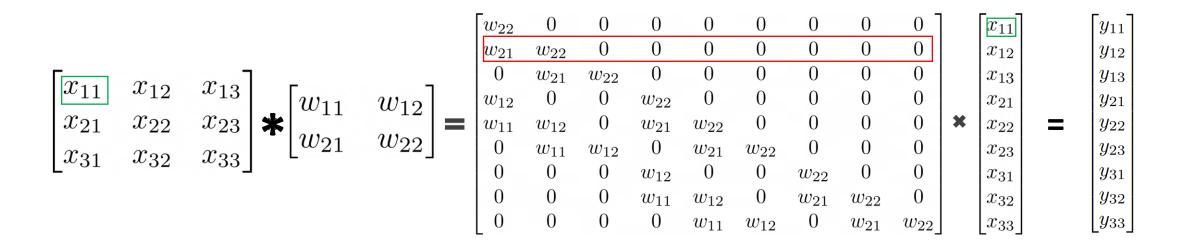
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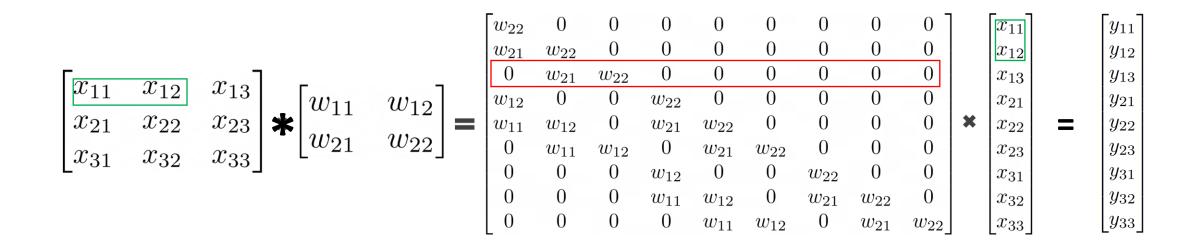




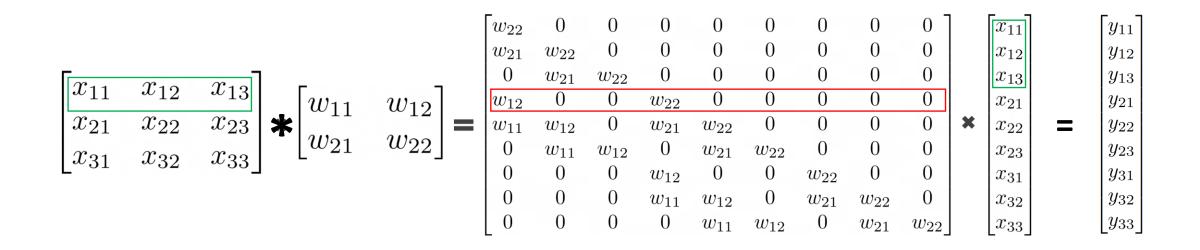
 $y_{11} = W_{22} z_{11}$



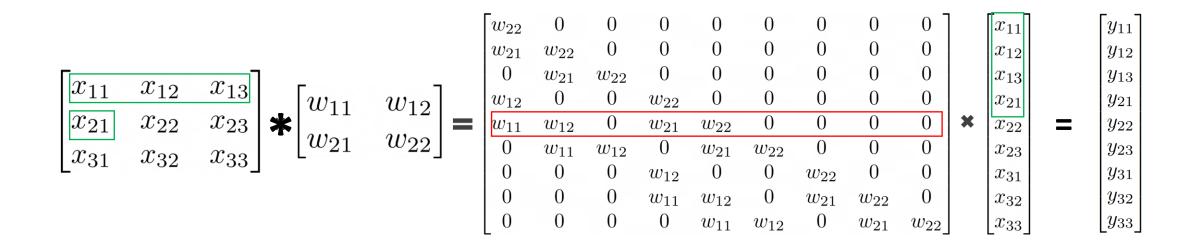
$$y_{12} = W_{21}\chi_{11} + W_{22}\chi_{12}$$



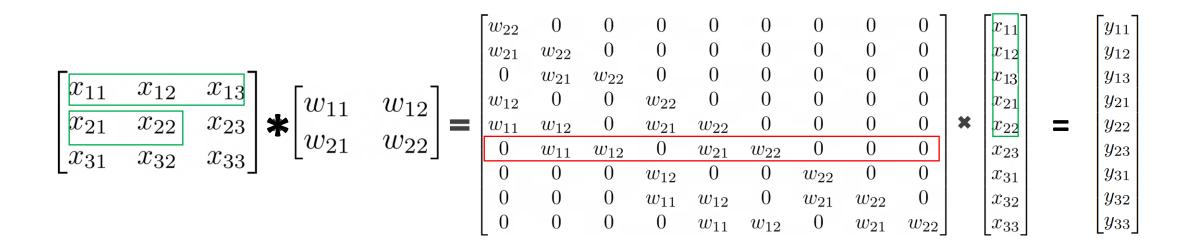
 $y_{13} = W_{21} \chi_{12} + W_{22} \chi_{13}$



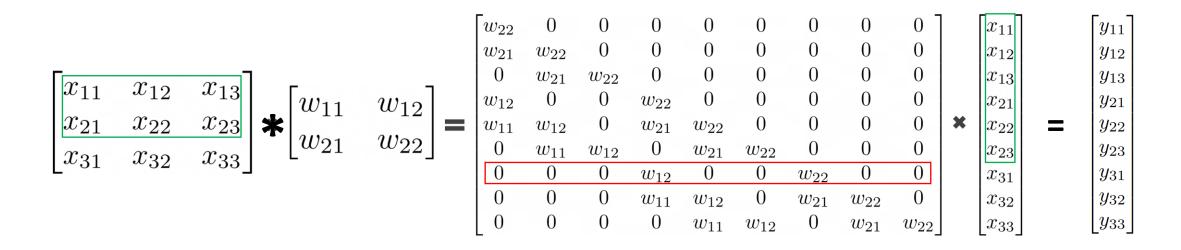
 $Y_{21} = W_{12} \chi_{11} + W_{22} \chi_{21}$



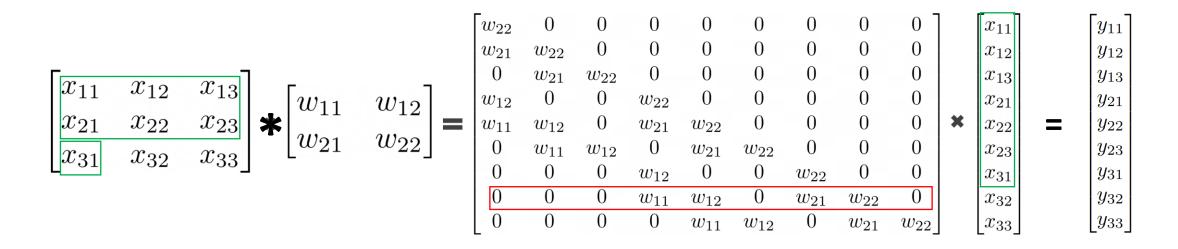
$$Y_{22} = W_{11} \chi_{11} + W_{12} \chi_{12} + W_{21} \chi_{21} + W_{22} \chi_{22}$$



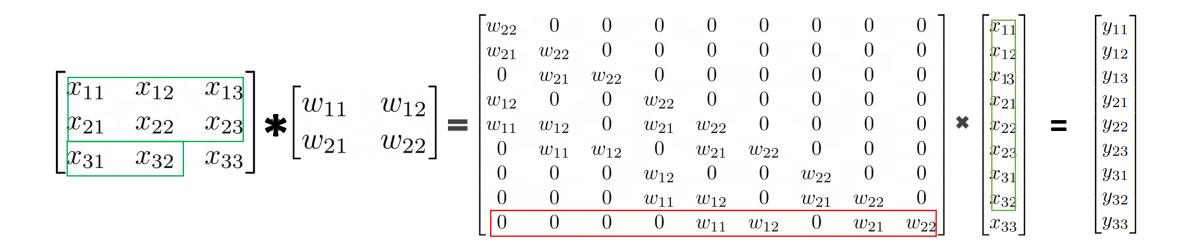
423 = WIINIZ + WIZNIZ + WZINZZ + WZZNZZ



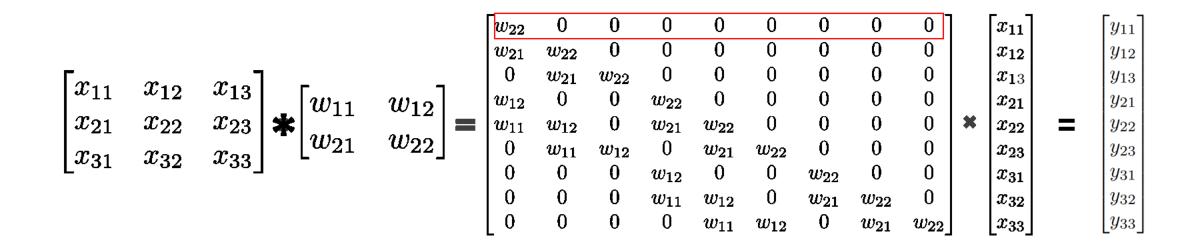
 $y_{31} = w_{12} x_{21} + w_{22} x_{31}$

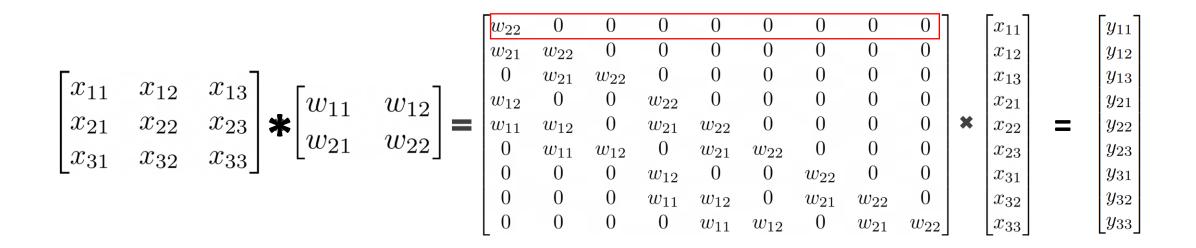


$$y_{32} = w_{11} x_{21} + w_{12} x_{22} + w_{21} x_{31} + w_{22} x_{32}$$

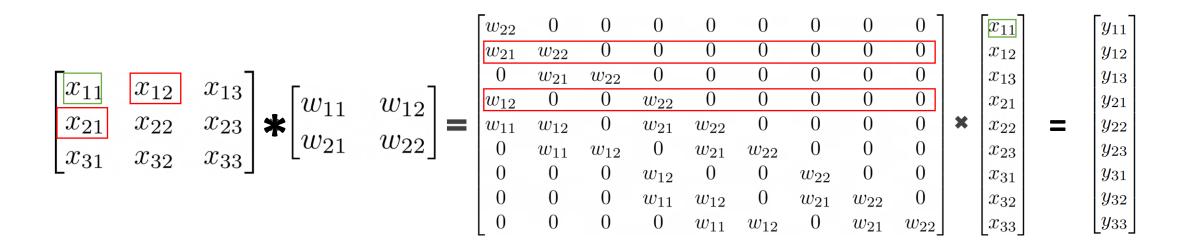


 $y_{33} = W_{11} \chi_{22} + W_{12} \chi_{23} + W_{21} \chi_{32} + W_{22} \chi_{33}$



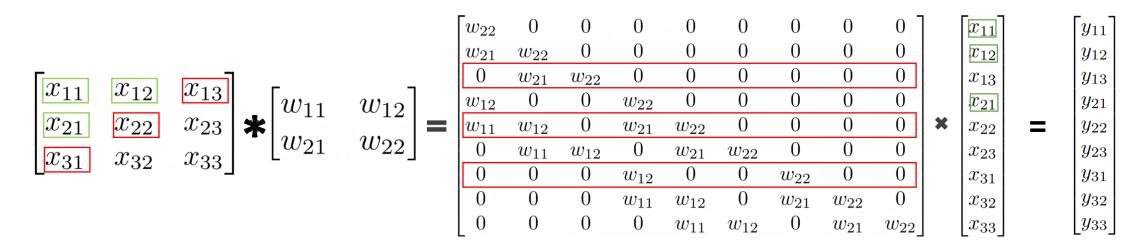


 $y_{11} = w_{22} x_{11}$

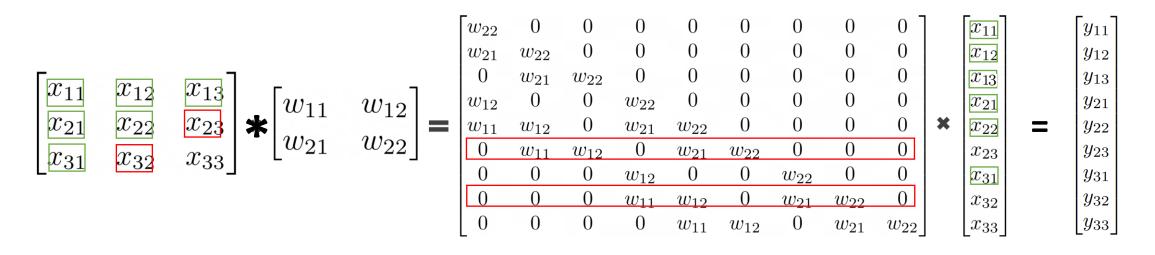


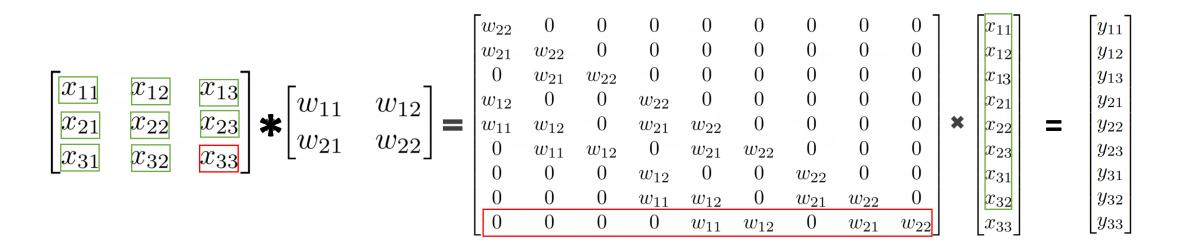
$$y_{12} = W_{21} \chi_{11} + W_{22} \chi_{12}$$

 $y_{21} = W_{12} \chi_{11} + W_{22} \chi_{21}$

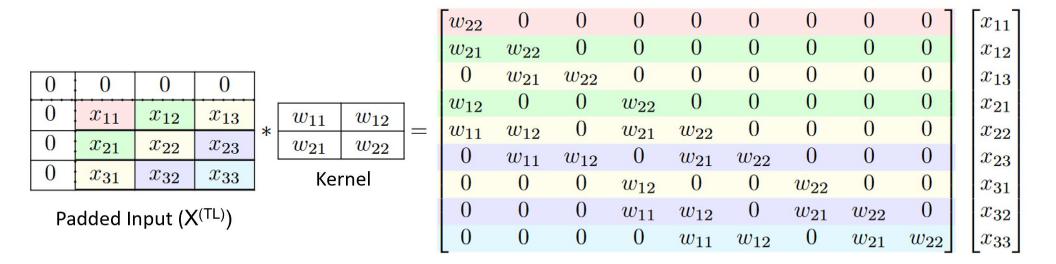


$$\begin{array}{rcl}
y_{13} &=& w_{21} \, \chi_{12} + w_{22} \, \chi_{13} \\
y_{22} &=& w_{11} \, \chi_{11} + w_{12} \, \chi_{12} + w_{21} \, \chi_{21} + w_{22} \, \chi_{22} \\
y_{31} &=& w_{12} \, \chi_{21} + w_{22} \, \chi_{31} \\
\end{array}$$





 $Y_{33} = W_{11} \chi_{22} + W_{12} \chi_{23} + W_{21} \chi_{32} + W_{22} \chi_{33}$



Convolution Matrix (**M**)

Vectorized Input(x)

x ₁₁	x ₁₂	x ₁₃	x ₁₄	x ₁₅	
x ₂₁	x ₂₂	x ₂₃	x ₂₄	x ₂₅	
x ₃₁	x ₃₂	x ₃₃	x ₃₄	x ₃₅	
x ₄₁	x ₄₂	x ₄₃	x ₄₄	x ₄₅	
x ₅₁	x ₅₂	x ₅₃	x ₅₄	x ₅₅	

*

w ₁₁	W ₁₂	W ₁₃
w ₂₁	w ₂₂	w ₂₃
W ₃₁	W ₃₂	W ₃₃

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Y ₁₁	¥12	Y ₁₃	Y ₁₄	¥15
y ₂₁	¥22	Y ₂₃	Y ₂₄	¥25
Y ₃₁	Y ₃₂	Y ₃₃	Y ₃₄	Y35
Y 41	Y ₄₂	Y ₄₃	Y 44	Y 45
Y51	¥52	Y53	¥54	Y55

_				
×15	x ₂₅	x ₃₅	x ₄₅	x ₅₅
×14	x ₂₄	x ₃₄	x 44	x ₅₄
x ₁₃	x ₂₃	x ₃₃	x ₄₃	x ₅₃
 x ₁₂	x ₂₂	x ₃₂	x ₄₂	x ₅₂
×11	x ₂₁	x ₃₁	x41	x ₅₁

*

w ₁₃	w ₂₃	W ₃₃
w ₁₂	w ₂₂	w ₃₂
W ₁₁	w ₂₁	w ₃₁

 Y15
 Y25
 Y35
 Y45
 Y55

 Y14
 Y24
 Y34
 Y44
 Y54

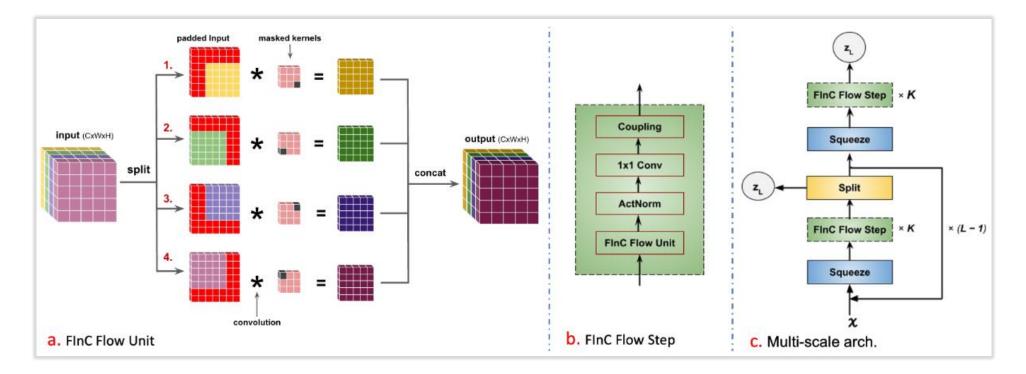
 Y13
 Y23
 Y33
 Y43
 Y53

 Y12
 Y22
 Y32
 Y42
 Y52

 Y11
 Y21
 Y31
 Y41
 Y51

FInC Flow

- Padding the input is done so that the resulting **M** is triangular
- Very minimal amount of masking required
- Inverse Time is O(nk²)



FINC Flow – Architecture

ActNorm

- Performs an affine transformation of the activations using a scale and bias parameter per channel, similar to batch normalization.
- Batch Normalization is not generally used because for large images, we need to train with batch_size = 1 and it creates a problem

$$egin{aligned} y_{i,j} = s \odot x_{i,j} + b \ x_{i,j} = rac{y_{i,j} - b}{s} \end{aligned}$$

FINC Flow – Architecture

Affine Coupling Layer

• A powerful reversible transformation where the forward function, the reverse function and the log-determinant are computationally efficient

$$egin{aligned} x_a, x_b &= ext{split}(x) \ (\log s, t) &= ext{NN}(x_b) \ s &= ext{exp}(\log s) \ y_a &= s \odot x_a + t \ y_b &= x_b \ y &= ext{concat}(y_a, y_b) \end{aligned}$$
 $egin{aligned} y_a, y_b &= ext{split}(y) \ (\log s, t) &= ext{NN}(y_b) \ s &= ext{exp}(\log s) \ x_a &= ext{exp}(\log s) \ x_a &= ext{exp}(\log s) \ x_b &= ext{yb} \ x &= ext{concat}(x_a, x_b) \end{aligned}$

FINC Flow – Architecture

Invertible 1x1 Convolution

 To incorporate a permutation along the channel dimension, we include a trainable invertible 1 × 1 convolution layer to generalize the permutation operation as:

$$egin{aligned} y_{i,j} &= W x_{i,j} \ x_{i,j} &= W^{-1} y_{i,j} \end{aligned}$$

Bijective Functions

Split

- Input is split into two halves across the channel dimension. We retain the first half and a
 function parameterized by first half transform the second half.
- The transformed second half is modeled as Gaussian samples, are the latent vectors.

Squeeze

• This function/layer reduces the feature dimension by total four, two across the height dimension and two across the width dimension resulting in increases the channel dimension by four

Theorem 1: The inverse of the pixels on the diagonals of a TL padded convolution can be computed independently and parallelly

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Proof: Because this is a TL padded convolution, $y_{i,j}$ depends only on the kxk window of $x_{\leq i, \leq j}$ $y_{i,i} = f(x_{\leq i, \leq j})$

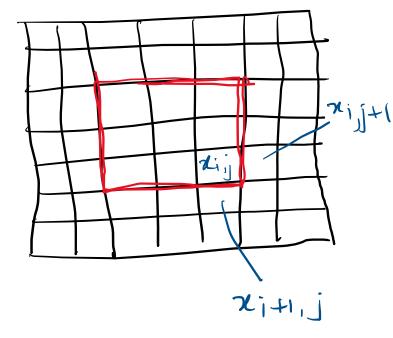
Theorem 1: The inverse of the pixels on the diagonals of a TL padded convolution can be computed independently and parallelly

Defn: Diagonal Elements: Let
$$\chi_{i,j} \notin \chi_{i',j'}$$
 be any two
elements of a matrix. Then $\chi_{i,j} \notin \chi_{i',j'}$ are said to be
on the same diagonal if $i+j = i'+j'$

Proof:
Because this is a TL podded convolution,
$$y_{i,j}$$
 depends only on
the KXK window of $x_{\leq i, \leq j}$
 $y_{i,i} = f(x_{\leq i, \leq j})$
 $x_{i,j} = \underbrace{y_{i,j} - f_1(x_{\leq i, < j})}_{W_{K,K}}$
 $x_{i,j} = \underbrace{y_{i,j} - f_1(x_{\leq i, < j})}_{W_{K,K}}$

1

$$\begin{aligned} \chi_{i+1,j} &= & \mathcal{Y}_{i+1,j} - f_{z}(\chi_{\langle i+1,j \rangle}) \\ &= & \mathcal{Y}_{i+1,j} - & \chi_{i,j} - f_{3}(\chi_{i+1,j-1},\chi_{i+1,j-2},...) \\ &- & f_{4}(\chi_{\langle i,\langle j \rangle}) \end{aligned}$$



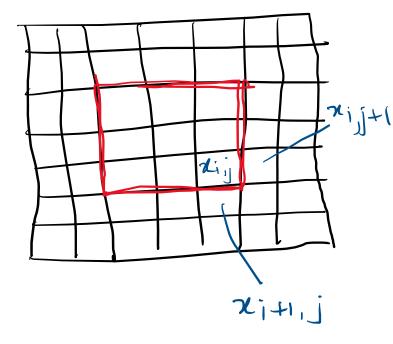
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$$\begin{aligned} \chi_{i+1,j} &= & Y_{i+1,j} - f_{z}(\chi_{ci+1,j}) \\ &= & Y_{i+1,j} - & \chi_{i,j} - f_{3}(\chi_{i+1,j-1},\chi_{i+1,j-2},...) \\ &- & f_{4}(\chi_{ci,cj}) \end{aligned}$$

But
$$z_{i,j} \& z_{i+i,j-1}$$
 can be computed independently
As is the case for $z_{i+1,j-2} \& z_{i,j-1} \& s_{\delta}$ on.

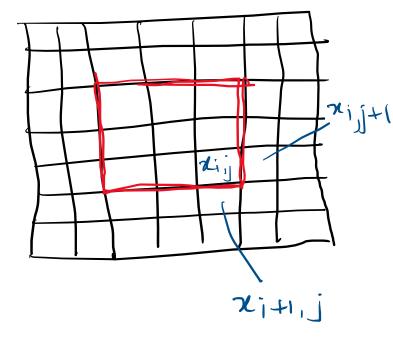


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$$\begin{aligned} \chi_{i+1,j} &= & y_{i+1,j} - f_2(\chi_{\langle i+1,j \rangle}) \\ &= & y_{i+1,j} - & \chi_{i,j} - f_3(\chi_{i+1,j-1},\chi_{i+1,j-2},...) \\ &- & f_4(\chi_{\langle i,\langle j \rangle}) \end{aligned}$$

But
$$z_{i,j} \& x_{i+i,j-1}$$
 can be computed independently
As is the case for $x_{i+1,j-2} \& z_{i,j-1} \& s_0 \text{ on}$.
So, $z_{i+1,j} = Y_{i+1,j} - K z_{i,j} - F_1(\text{remaining pixels})$
 III^{IY} , $z_{i,j+1} = Y_{i,j+1} - \beta z_{i,j} - F_2(\text{remaining pixels})$



Algorithm 1: Fast Parallel Inverse Algorithm for a TL Padded Convolution Block

```
Input: K: Kernel of shape (C, C, k_H, k_W)
Y: output of the conv of shape (C, H, W)
Result: X: inverse of the conv. with shape (C, H, W).
Initialization: X \leftarrow Y;
for d \leftarrow 0, H + W - 1 do
   for c \leftarrow 0, C-1 do
       /* The below lines of code executes parallelly on different
           threads on GPU for every index (c, h, w) of X on the dth
           diagonal.
                                                                                      */
       for k_h \leftarrow 0, k_H - 1 do
          for k_w \leftarrow 0, k_W - 1 do
              for k_c \leftarrow 0, C-1 do
                  if pixel (k_c, h - k_h, w - k_w) not out of bounds then
                    X[c,h,w] \leftarrow
                     X[c,h,w] - X[k_c,h-k_h,w-k_w] * K[c,k_c,k_H-k_h-1,k_W-k_w-1];
                  end
              end
          \mathbf{end}
       end
       /* synchronize all threads
                                                                                      */
   end
end
```

Theorem 2: Algorithm 1 uses only $(H + W - 1)k^2$ sequential operations.

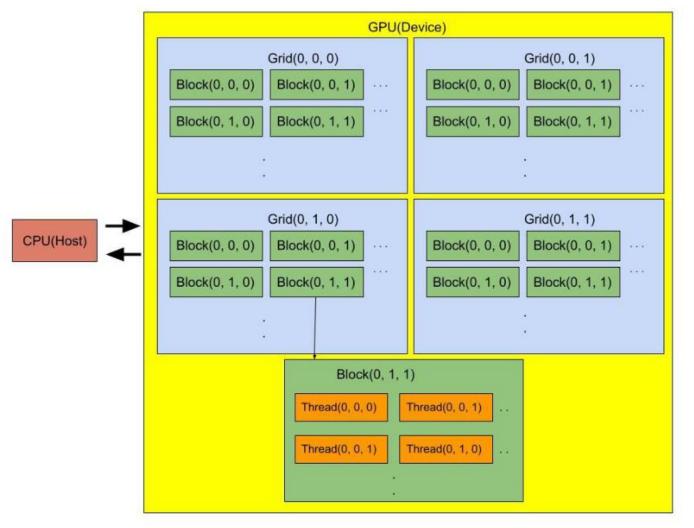
Proof:

We have proved in Theorem 1 that the inverse of pixels on a single diagonal can be computed parallelly in one iteration of Algorithm 1. Since there are H + W - 1 number of diagonals in a matrix and there are at maximum k^2 entries in a row of the convolutional matrix, the number of sequential operations needed will be $(H + W - 1)k^2$.

Algorithm 2: Fast Inverse Algorithm for FInC Flow Unit

- **Input:** K_1, K_2, K_3, K_4 Convolution Kernels of different PCB, Y Output of the FInC Flow Unit
- **Result:** X Input to the FInC Flow Unit / Inverse of the FInC Flow Unit
 - 1. $Y_1, Y_2, Y_3, Y_4 \leftarrow split(Y)$
 - 2. Flip $Y_2, Y_3, Y_4, K_2, K_3, K_4$ (inplace) appropriately to match TL padding
 - 3. $X \leftarrow concat(Y_1, Y_2, Y_3, Y_4)$
 - 4. $K \leftarrow concat(K_1, K_2, K_3, K_4)$
 - 5. Apply Algorithm 1 with input K, Y to get X
 - 6. $X_1, X_2, X_3, X_4 \leftarrow split(X)$
 - 7. Flip X_2, X_3, X_4 appropriately to get the correct output
 - 8. $X \leftarrow concat(X_1, X_2, X_3, X_4)$

GPU (CUDA) - Architecture



CUDA Architecture

CUDA - Programming

A typical execution of a CUDA C/C++ code involves several steps like

- 1. Allocate memory on the host for input and output
- 2. Allocate memory on the device(GPU)
- 3. Copy data from host to device
- 4. Launch the kernel CUDA function and execute it
- 5. Copy the results back to host
- 6. Free the memory on both the host and the device

CUDA - Programming

int tid = threadIdx.x + blockDim.x * (threadIdx.y + blockDim.y * threadIdx.z);

ThreadID Calculation Code

int bid = blockIdx.x + gridDim.x * (blockIdx.y + gridDim.y * blockIdx.z);

BlockID Calculation Code

Algorithm 1 Code: Link Algorithm 2 Code: Link

CUDA – Main Function

```
for (int d = 1; d <= H + W - 1; d++) { // Iterating over diagonal index
   for (int c = 0; c < C; c++) {
       // all elements of the dth diagonal computed in parallel
       int relevant threads = d;
       if (d > H) {
           if (d <= W) {
               relevant threads = H;
            } else {
                relevant threads = H + W - d;
       dim3 threads(B, 1, 1);
        dim3 blocks (relevant threads, 1, 1);
       AT_DISPATCH_FLOATING_TYPES(input.type(), "finc_inverse_cuda", ([&] {
            cinc cuda inverse kernel<scalar t><<<blocks, threads>>>(
                input.packed accessor<scalar t, 4, torch::RestrictPtrTraits,size t>(),
                kernel.packed accessor<scalar t, 4, torch::RestrictPtrTraits,size t>(),
                output.packed accessor<scalar t, 4, torch::RestrictPtrTraits, size t>(),
                c,
                d,
                relevant threads
            );
        }));
       cudaDeviceSynchronize();
```

CUDA – Kernel

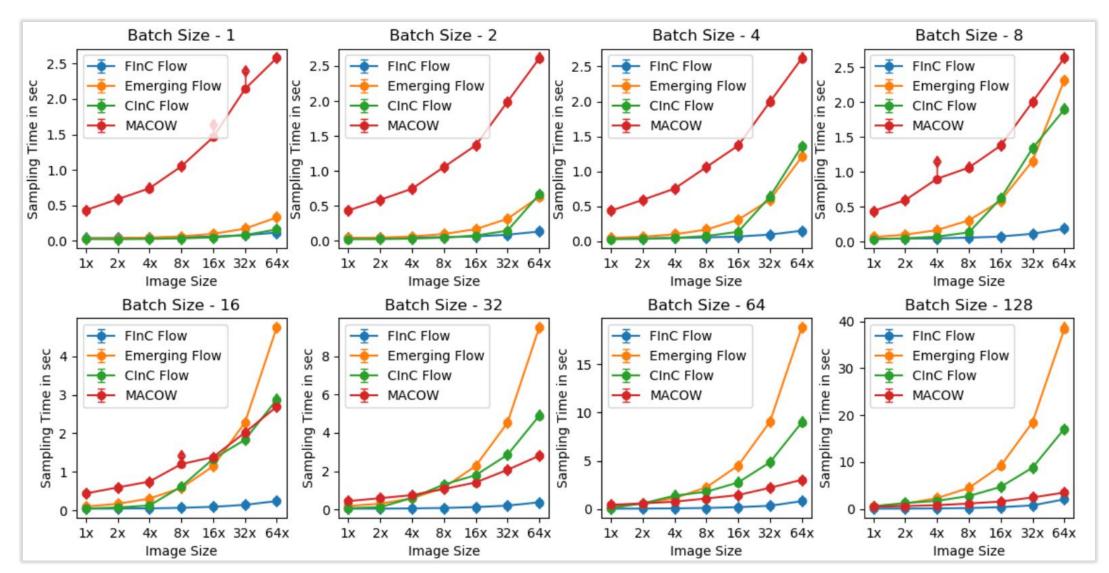
```
const auto tid = blockIdx.x;
const auto b = threadIdx.x;
int h, w, n = H;
// h = tid % m; // batch index encoded in lower indices modulo batchsize
// tid = (tid - h) / m; // remaining part of tid has the index along the diagonal
if (d <= n) {
   h = d - 1 - tid;
   w = tid;
} else {
   w = (d - n) + tid;
   h = n - 1 - tid;
// compute entry of the output in the diagonal d assigned to this thread
output[b][c][h][w] = input[b][c][h][w];
for (int k h = 0; k h < K H; k h++) {
    if (h - k h < 0) break;
    for (int \overline{k} w = 0; k w < K W; k w++) {
        if (w - k w < 0) break;
        for (int k = 0; k < C; k < ++) {
            if (kh == 0 \& kw == 0) {
                if (k c == c) continue;
            output[b][c][h][w] -= output[b][k c][h - k h][w - k w] * kernel[c][k c][K H - k h - 1][K W - k w - 1];
```

Comparison of BPD, FT, ST with other Convolution Based Models

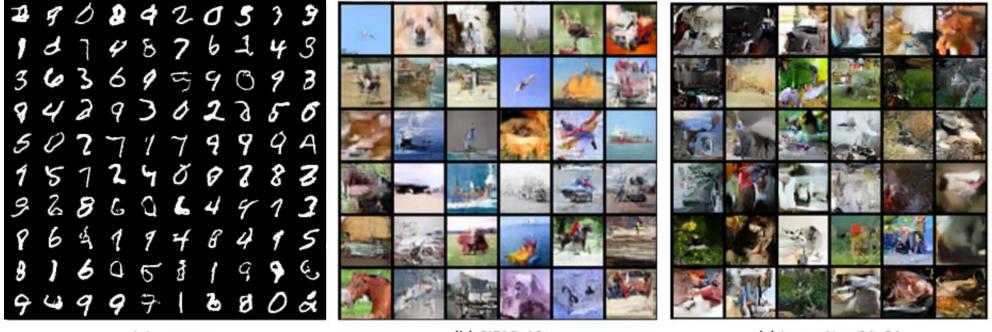
- Datasets Used:
 - MNIST
 - CIFAR-10
 - Imagenet 32x32
 - Imagenet 64x64

Model	MNIST		CIFAR-10		Imagenet-32x32		Imagenet-64x64					
	BPD	FT	ST	BPD	FT	ST	BPD	FT	ST	BPD	FT	ST
Emerging	_	0.16	0.62	3.34	0.49	17.19	4.09	0.73	25.79	3.81	1.71	137.04
MaCow	_	_	_	3.16	1.49	3.23	_	_	_	3.69	2.91	8.05
CInC Flow	_	_	_	3.35	0.42	7.91	4.03	0.62	11.97	3.85	1.57	55.71
MintNet	0.98	0.16	17.29	3.32	2.09	230.17	4.06	2.08	230.44	_	_	_
FInC Flow (our)	1.05	0.14	0.09	3.39	0.37	0.41	4.13	0.48	0.52	3.88	1.43	2.11

Comparison of Sample Times with other models



Generate Samples

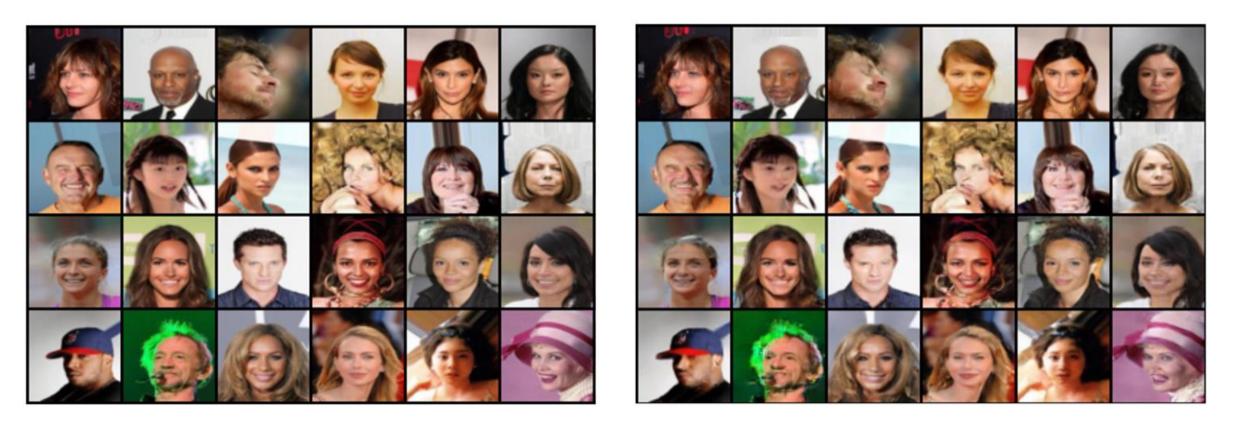


(a) MNIST

(b) CIFAR-10

(c) ImageNet-64x64

Image Reconstruction



Reconstructed Images

Input Images

Dataset	(L, K)	#Params	#Samples	Algorithm 1 ST	Algorithm 2 ST	
MNIST	(2, 16)	10 M	1	0.09	0.07	
MNIST	(2, 16)	10 M	100	0.12	0.09	
CIFAR10	(3, 32)	45M	1	0.73	0.30	
CIFAR10	(3, 32)	45M	100	0.92	0.47	
Imagenet32	(4, 48)	67M	1	1.01	0.44	
Imagenet32	(4, 48)	67M	100	1.38	0.73	
Imagenet64	(3, 32)	45M	1	1.42	0.50	
Imagenet64	(3, 32)	45M	100	2.31	1.42	

Comparison of Algorithm 1 and Algorithm 2

Conclusion

With a parallel inversion approach, we present a k × k invertible convolution for Normalizing flow models. We utilize it to develop a model with highly efficient sampling pass, normalizing flow architecture. We implement our parallel algorithm on GPU and presented benchmarking results, which show a significant enhancement in forward and sampling speeds when compared to alternative methods for k × k invertible convolution

Any Questions?



https://github.com/aditya-v-kallappa/FInCFlow