Analysis of SVD Deep Neural Network parametrization

“Da kto takoi etot et al?!” team

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Theoretical Part

Problem

Time consuming operations!

Neural Networks →

1) Matrix inversion
2) Matrix Determinant
3) Spectral normalizations

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Solution →

SVD decomposition

$$W = U\Sigma V^T$$

Σ - diagonal
U, V - orthogonal

What is the problem? →

Gradient Descent Update of Weight Matrix

$$\Sigma' = \Sigma - \eta\nabla_\Sigma$$

$$U' = U - \eta\nabla_U$$

$$V' = V - \eta\nabla_V$$

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$\xrightarrow{\text{Solution}}$ SVD decomposition

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Neural Networks $\longrightarrow$

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Solution $\longrightarrow$

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Loss of orthogonality of U, V matrices

Theoretical Part

To preserve U, V orthogonality:

$$U \in \mathbb{R}^{d\times d}$$

Householder matrices

$$U = \prod_{i=1}^{d} H_i \qquad H_i = I - 2\frac{v_i v_i^T}{||v_i||_2^2} \qquad v_i \in \mathbb{R}^d.$$

All products of Householder matrices are orthogonal → Any dxd orthogonal matrix can be decomposed as a product of *d* Householder matrices → Allows to perform gradient descent over orthogonal matrices

Why Householder matrices are good?

- U **remains orthogonal** under gradient descent update at *i* step
- It allows to perform gradient descent to **preserve the SVD** of W during gradient descent updates

What is the FastH algorithm?

Need to calculate:

$$UX = H_1 \cdots (H_{d-1}(H_d \cdot X))$$
$$X \in \mathbb{R}^{d \times m}$$

- Sequential

$$O(d^2 m)$$

$O(d)$ sequential vector-vector operations

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- FastH

$$\boxed{O(d^2m)}$$

$O(\frac{d}{m} + m)$ sequential matrix operations

FastH. Forward Pass

Input: $X \in \mathbb{R}^{d \times m}, \ d > m > 1$

$H_1, \ldots, H_d \ , \ H_i \in \mathbb{R}^{d \times d}$ - Householder matrices

Want to compute: $A = H_1 \cdots H_d X$

$$H_i = I - \frac{2 v_i v_i^T}{\|v_i\|_2^2} \ , \qquad P_i = \underbrace{H_{(i-1)\cdot m+1} \cdots H_{i \cdot m}}_{m \text{ matrices}} \quad i = 1, \ldots, \frac{d}{m}$$

Then: $A = \underbrace{H_1 \cdots H_d}_{d \text{ multiplications}} X = \underbrace{P_1 \cdots P_{\frac{d}{m}}}_{\frac{d}{m} \text{ multiplications}} X$

$P_i X$ takes $O(d^2 m)$
Then compute A
takes $O(d^3)$

Still slow.... :c

Using decomposition of product ~ $O(dm^2)$

$H_1 \cdots H_m = I - 2WY^T$

helps us reduce complexity of computation to $O(d^2 m)$
and decrease number of matrix multiplication to $O(\frac{d}{m} + m)$

FastH. Backwards Propagation

Input: $A_1, \ldots, A_{\frac{d}{m}+1}, P_1, \ldots, P_{\frac{d}{m}+1}, \dfrac{\partial L}{\partial A_1}$ L - loss function

Want to compute: $\dfrac{\partial L}{\partial X}, \dfrac{\partial L}{\partial v_1}, \ldots, \dfrac{\partial L}{\partial v_d}$

The backward pass of FastH has two steps:

1. Compute $\dfrac{\partial L}{\partial A_2}, \dfrac{\partial L}{\partial A_3}, \ldots, \dfrac{\partial L}{\partial A_{\frac{d}{m}+1}}$ by $\dfrac{\partial L}{\partial A_{i+1}} = \left[\dfrac{\partial A_i}{\partial A_{i+1}}\right]^T \dfrac{\partial L}{\partial A_i} = P_i^T \dfrac{\partial L}{\partial A_i}$ $\longrightarrow$ gradient wrt. X since $X = A_{\frac{d}{m}+1}$

2. Compute $\dfrac{\partial L}{\partial v_j}$ for all j $\rightarrow$ can be split into d/m subproblems $\rightarrow$ can be solved in parallel $\rightarrow$ one subproblem for each $\dfrac{\partial L}{\partial A_i}$

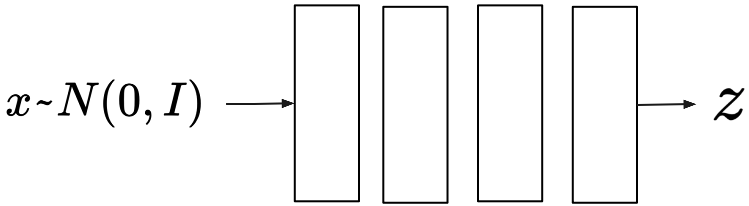
Applications

- Normalization flow models
  - Matrix determinant
  - Inverse matrix
- Spectral normalization

Normalization flow

What do we want?

simple distributions $\xrightarrow{\text{map}}$ complex distributions



How?

By a sequence of invertible and differentiable mappings

Change of variables

$$p_X(\mathbf{x}) = p_Z\left(f^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial f^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

For invertible matrix:

$$p_X(\mathbf{x}) = p_Z(\mathbf{z})\left|\det\left(\frac{\partial f(\mathbf{z})}{\partial \mathbf{z}}\right)\right|^{-1}$$

1. $f(x)$ has to be invertible
2. want fast calculation of determinant of Jacobian matrix

$$det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)$$

Flow-based Generative Models

x - a high-dimensional random vector, collect a dataset D

generative process

$z \sim p_\theta(z)$

$x = g_\theta(z)$

f is composed of a sequence of transformations

$f = f_1 \circ f_2 \circ \ldots \circ f_K$

$$\mathbf{x} \overset{\mathbf{f}_1}{\longleftrightarrow} \mathbf{h}_1 \overset{\mathbf{f}_2}{\longleftrightarrow} \mathbf{h}_2 \cdots \overset{\mathbf{f}_K}{\longleftrightarrow} \mathbf{z}$$

normalizing flow

Normalizing flows are generative models which produce tractable distributions.

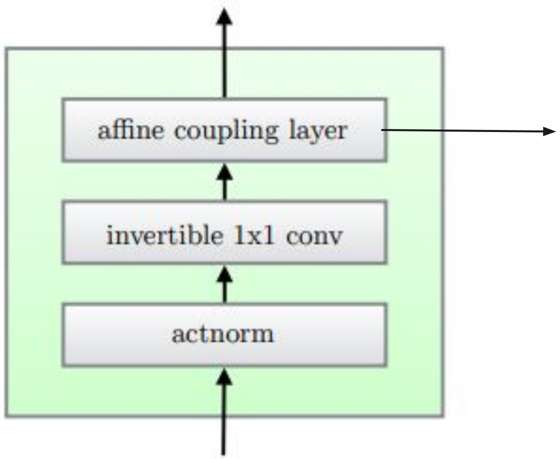
The probability density function of the model given a datapoint:

$$\boxed{\begin{aligned}\log p_{\boldsymbol{\theta}}(\mathbf{x}) &= \log p_{\boldsymbol{\theta}}(\mathbf{z}) + \log|\det(d\mathbf{z}/d\mathbf{x})| \\ &= \log p_{\boldsymbol{\theta}}(\mathbf{z}) + \sum_{i=1}^{K} \log|\det(d\mathbf{h}_i/d\mathbf{h}_{i-1})|\end{aligned}}$$

The log-determinant is the change in log-density when going from h_{i-1} to h_i under transformation f_i.

Glow: Generative Flow

Generative flow where each step



$$(x_a, x_b) \mapsto (y_a, y_b)$$

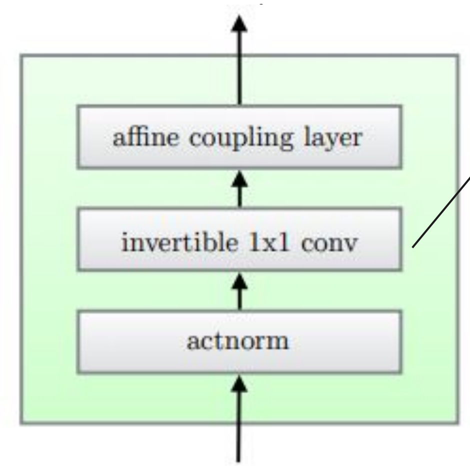
$$y_a = x_a$$

$$y_b = s(x_a) \odot x_b + t(x_a)$$

$$det\left(\frac{dy}{dx}\right) = det\begin{pmatrix} I & 0 \\ \frac{dy_a}{dx_a} & \frac{dy_b}{dx_b} \end{pmatrix} = det\left(\frac{dy_b}{dx_b}\right)$$

Glow: Generative Flow

Generative flow
where each step



$$y_{ij} = W x_{ij}$$
$$x_{ij} \in \mathbb{R}^d, W \in \mathbb{R}^{d \times d}$$

Log-determinant

$$det(\frac{dy}{dx}) = h \cdot w \cdot log|det(W)|$$

$$W = PL(U + \text{diag}(s))$$

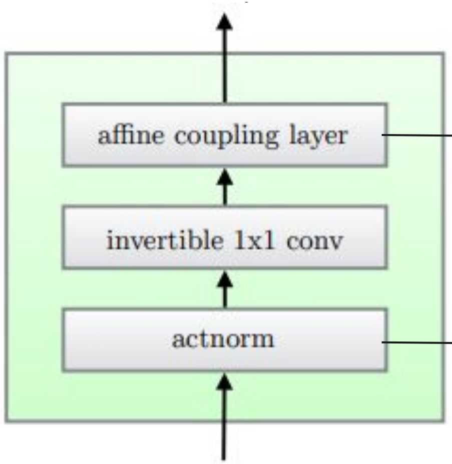
or

$$\boxed{W = U \Sigma V^T}$$

Can use FastH(SVD) here

Glow: Generative Flow

Generative flow
where each step



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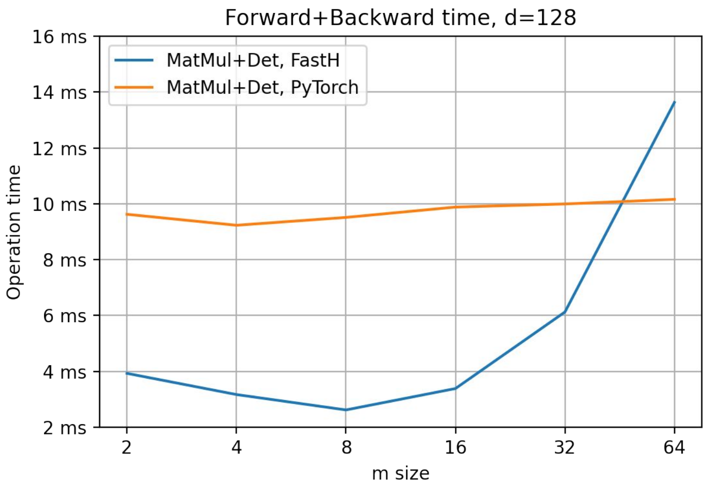
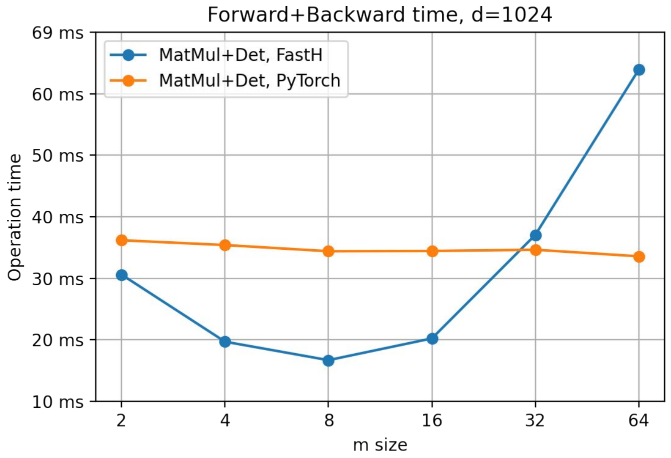
$$\forall i, j : \mathbf{y}_{i,j} = \mathbf{s} \odot \mathbf{x}_{i,j} + \mathbf{b}$$

$$det\left(\frac{dy}{dx}\right) = h \cdot w \cdot \mathrm{sum}(\log|\mathbf{s}|)$$

How we can use FastH(SVD) here





How we can use FastH(SVD) here

Efficient FastH operation: $UX, U \in \mathbb{R}^{d\times d}, X \in \mathbb{R}^{d\times m}$

But! By algorithm formulation $\boldsymbol{m} \ll \boldsymbol{d}$

For conv 1x1 $X \in \mathbb{R}^{d\times BHW}$

B - batch size
H - height
W - width

$\Rightarrow$ $\boldsymbol{m} \gg \boldsymbol{d}$

Can not be applied straightforwardly!

How we can use FastH(SVD) here

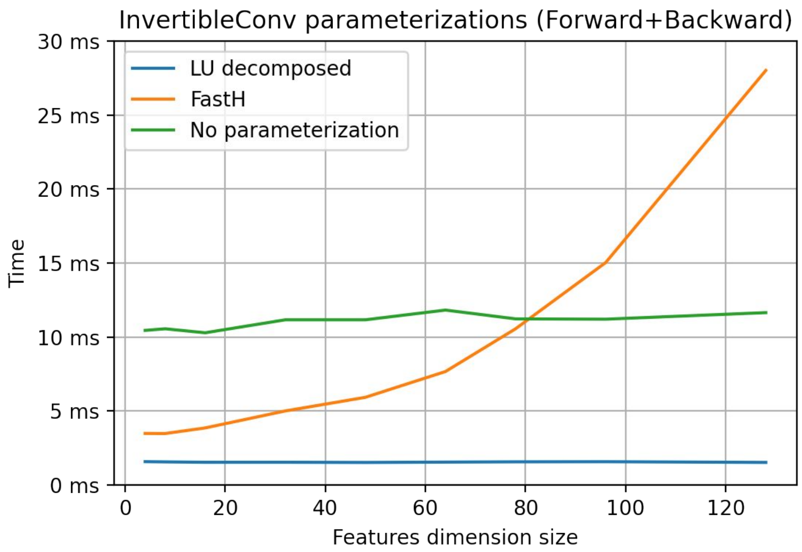
Alternative: 1) extract weight matrix:

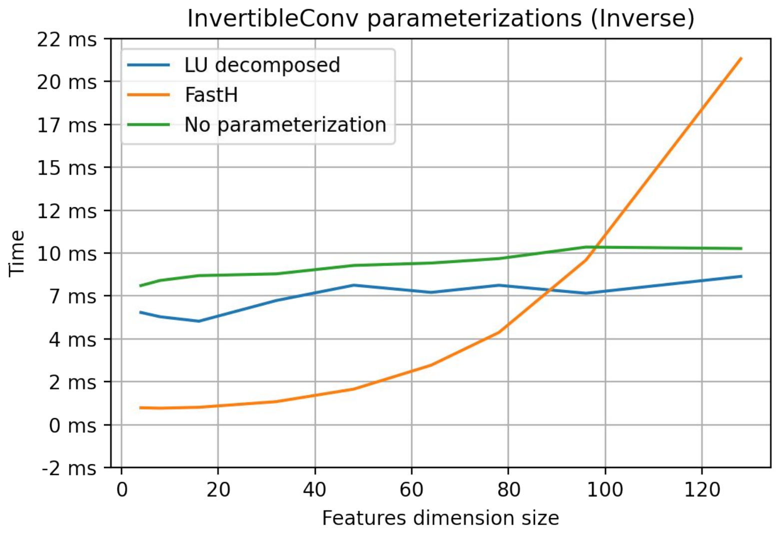
$$W = \begin{bmatrix} U \begin{pmatrix} I_{d/2} \\ 0 \end{pmatrix} \\ U \begin{pmatrix} 0 \\ I_{d/2} \end{pmatrix} \end{bmatrix}$$

using two FastH forwards

2) Apply 2D 1x1 convolution using W matrix

How we can use FastH(SVD) here





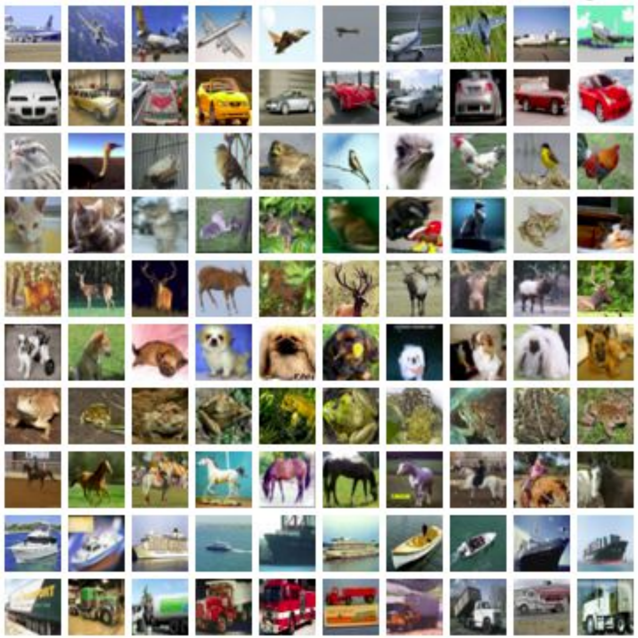
GLOW performance

	Pytorch	FastH
Forward	160 ms	**112 ms**
Inverse	475 ms	**113 ms**
Forward+Backward	513 ms	**245 ms**

~7.5 min (out of 15) per epoch reduction!
(CIFAR10)

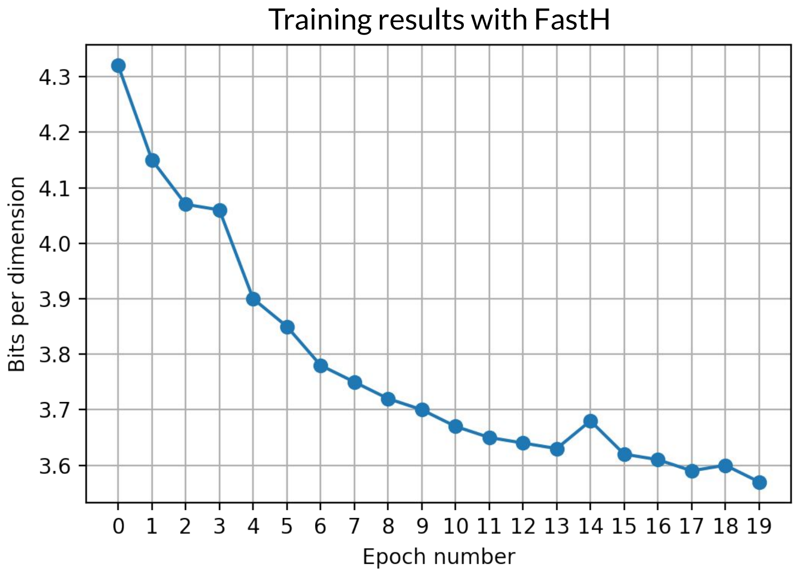
CIFAR-10

Real examples



After 20 epochs

CIFAR-10



$$BPD = \frac{NLL}{3 \ln 2 \cdot H \cdot W}$$

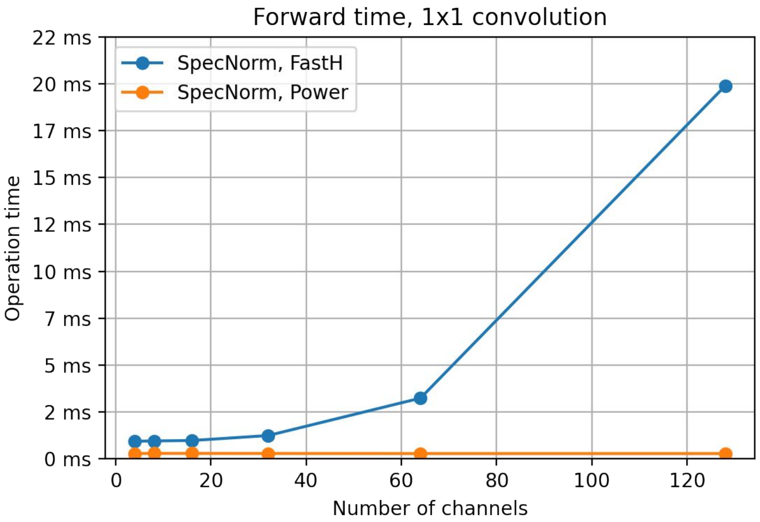
➔ After 20 epochs: **3.57 bpd**

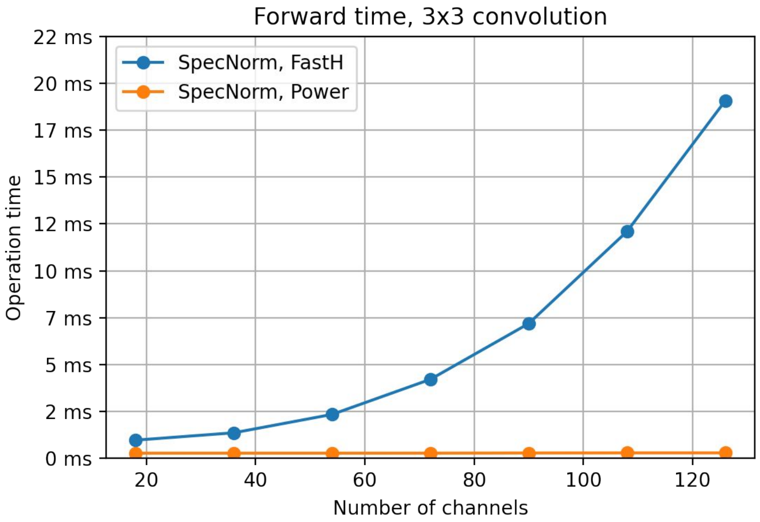
➔ For original GLOW should be ~3.48 after 80 epochs

It works!

Spectral normalization

$$W \in \mathbb{R}^{C_{out} \times C_{in} \times K \times K} \qquad \sigma(W) \to 1$$





Conclusion

- ➔ Practical speed-up can be achieved for GLOW model

BUT:

- ➔ A lot of limitations on parameters choice
- ➔ There is more powerful models (e.g. Neural Splines Flow)
- ➔ The only normalization flow model can be accelerated?

Spectral norms:

- ➔ Slower than power iteration