ASDL: A Unified Interface for Gradient Preconditioning in PyTorch

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NEURAL INFORMATION PROCESSING SYSTEMS

Gradient Preconditioning in Deep Learning

Gradient-based optimization

$$\underbrace{\theta_{t+1}}_{\text{Parameter}} \leftarrow \theta_t - \eta \overbrace{\underbrace{P_t}_{\text{Preconditioning matrix}} \underbrace{g_t}_{\text{Gradient}}}^{\textbf{Preconditioned gradient}}$$

How to deal with nonconvexity, stochasticity, and high dimensionality in Deep Learning?

Background & problem: A diverse set of gradient preconditioning methods

1. Curvature matrix C

- **Loss sharpness**
  - Hessian H
  - Absolute Hessian $H_{|\lambda|}$
  - BFGS Hessian H_{bfgs}
  - Gauss-Newton matrix G
- **Gradient covariance**
  - Fisher information matrix F
  - FIM est. by MC samples $\hat{F}_{n\mathrm{mc}}$
- **Gradient 2nd moment**
  - Empirical Fisher $\hat{F}_{\mathrm{emp}}$
  - Batched empirical Fisher $\hat{F}^{\mathrm{batch}}_{\mathrm{emp}}$

2. Representation of C

- **Full**
  - Dense/sparse/low-rank
  - Matrix-free/Gram
- **Layer-wise** (block-diagonal)
  - Dense/sparse/low-rank
  - Gram/Kronecker-factored
- **Unit-wise** (block-diagonal)
  - Dense/sparse/low-rank
  - Gram
- **Element-wise** (diagonal)
  - Dense/sparse

3. Solver for $Pg \approx C^{-1}g$

- **Local iterative** (matrix-free)
  - Conjugate gradient
  - Krylov subspace
  - Neumann series
- **Global iterative**
  - BFGS
  - Learning by SGD
- **Local/global direct**
  - Cholesky inverse/solve
  - Eigendecomposition
  - SMW formula

"KF-io": input-output Kronecker-factored. "KF-dim": dimension-wise Kronecker-factored. "RR": rank reduction. "SMW": Sherman-Morrison-Woodbury formula. "L": local = one mini-batch at one time step. "G": global = multiple mini-batches at multiple time steps. "iter": iterative.

Method	1. Curvature matrix C		2. Representation of C		3. Solver for $Pg \approx C^{-1}g$	
	type	matrix	granularity	format	type	key operations
LiSSA (Agarwal et al., 2017)	sharpness	H	full	dense	G iter	Neumann series
PSGD (Li, 2018)	sharpness	$H_{\lvert\lambda\rvert}$	full	dense	G iter	triangular solve & SGD
Neumann optimizer (Krishnan et al., 2017)	sharpness	H	full	matrix-free	L iter	Neumann series
Hessian-free (Martens, 2010)	sharpness	H, G	full	matrix-free	L iter	conjugate gradient
KSD (Vinyals & Povey, 2011)	sharpness	H, G	full	matrix-free	L iter	Krylov subspace method
L-BFGS (Liu & Nocedal, 1989)	sharpness	H_{bfgs}	full	matrix-free	G iter	approx. BFGS
SMW-GN (Ren & Goldfarb, 2019)	sharpness	G	full	Gram, RR	L direct	SMW inverse
SMW-NG (Ren & Goldfarb, 2019)	grad 2^{nd}m	$\hat{F}_{\mathrm{emp}}$	full	Gram, RR	L direct	SMW inverse
TONGA (Roux et al., 2008)	grad 2^{nd}m	$\hat{F}_{\mathrm{emp}}$	full	Gram, RR	G direct	SMW solve & eigendecomp.
M-FAC (Frantar et al., 2021)	grad 2^{nd}m	$\hat{F}^{\mathrm{batch}}_{\mathrm{emp}}$	full	Gram, RR	G direct	SMW solve
GGT (Agarwal et al., 2019)	grad 2^{nd}m	$(\hat{F}^{\mathrm{batch}}_{\mathrm{emp}})^{1/2}$	full	Gram, RR	G direct	SMW solve
FANG (Grosse & Salakhutdinov, 2015)	grad cov	$\hat{F}_{n\mathrm{mc}}$	full	sparse	L/G direct	incomplete Cholesky
★ PSGD (KF) (Li, 2018)	sharpness	$H_{\lvert\lambda\rvert}$	layer	KF-io	G iter	triangular solve & SGD
★ K-BFGS (Goldfarb et al., 2021)	sharpness	H_{bfgs}	layer	KF-io	G iter	BFGS
★ K-FAC (Martens & Grosse, 2015)	grad cov, 2^{nd}m	$\hat{F}_{n\mathrm{mc}}, \hat{F}_{\mathrm{emp}}$	layer	KF-io	L/G direct	Cholesky inverse
KFLR (Botev et al., 2017)	grad cov	F	layer	KF-io	L/G direct	Cholesky inverse
KFRA (Botev et al., 2017)	grad cov, 2^{nd}m	$\hat{F}_{n\mathrm{mc}}, \hat{F}_{\mathrm{emp}}$	layer	KF-io	L/G direct	Cholesky inverse & recursion
EKFAC (George et al., 2018)	grad cov, 2^{nd}m	$\hat{F}_{\mathrm{emp}}$	layer	KF-io	L/G direct	eigendecomp. (or SVD)
SKFAC (Tang et al., 2021)	grad cov, 2^{nd}m	$\hat{F}_{1\mathrm{mc}}, \hat{F}_{\mathrm{emp}}$	layer	KF-io, RR	L direct	SMW inverse & reduction
★ SENG (Yang et al., 2021)	grad 2^{nd}m	$\hat{F}_{\mathrm{emp}}$	layer	Gram, RR	L/G direct	SMW inverse & sketching
TNT (Ren & Goldfarb, 2021)	grad cov, 2^{nd}m	$\hat{F}_{n\mathrm{mc}}, \hat{F}_{\mathrm{emp}}$	layer	KF-dim	L direct	Cholesky inverse
★ Shampoo (Gupta et al., 2018)	grad 2^{nd}m	$(\hat{F}^{\mathrm{batch}}_{\mathrm{emp}})^{1/2}$	layer	KF-dim	G direct	eigendecomp.
unit-wise NG (Ollivier, 2015)	grad cov, 2^{nd}m	$\hat{F}_{n\mathrm{mc}}, \hat{F}_{\mathrm{emp}}$	unit	dense	L/G direct	Cholesky inverse
TONGA (unit) (Roux et al., 2008)	grad 2^{nd}m	$\hat{F}_{\mathrm{emp}}$	unit	Gram, RR	G direct	SMW solve & eigendecomp.
AdaHessian (Yao et al., 2020b)	sharpness	$H_{\lvert\lambda\rvert}$	element	dense	G direct	element-wise division
SFN (Dauphin et al., 2014)	sharpness	$H_{\lvert\lambda\rvert}$	element	dense	L/G direct	element-wise division
Equilibrated SGD (Dauphin et al., 2015)	sharpness	$H_{\lvert\lambda\rvert}$	element	dense	L/G direct	element-wise division
AdaGrad (Duchi et al., 2011)	grad 2^{nd}m	$(\hat{F}^{\mathrm{batch}}_{\mathrm{emp}})^{1/2}$	element	dense	G direct	element-wise division
Adam (Kingma & Ba, 2015)	grad 2^{nd}m	$(\hat{F}^{\mathrm{batch}}_{\mathrm{emp}})^{1/2}$	element	dense	G direct	element-wise division

★: methods to be analyzed in this study

✗ Each requires algorithm-specific and complex implementations.

✗ The compute performance, prediction accuracy, and feasibility (time and memory) are highly dependent on neural network architectures and specific training settings.

Automatic Second-order Differentiation Library (ASDL)

Our solution: A unified interface by ASDL

✓ ASDL offers various implementations and a unified interface for gradient preconditioning in PyTorch (an automatic-differentiation library).

✓ ASDL enables an easy integration of gradient preconditioning into a training with procedures that are algorithm-independent and as simple (same logical structure) as the standard training pipeline (see the figure on the right.)

✓ ASDL works with arbitrary deep neural networks defined with basic building blocks (e.g., nn.Linear, nn.Conv2d, nn.BatchNormNd, nn.LayerNorm, nn.Embedding) in PyTorch.

ASDL enables flexible switching and structured comparison of gradient preconditioning methods in DL

Standard training pipeline in PyTorch

```
for x, t in data_loader:
  optimizer.zero_grad()

  # Compute mini-batch gradient g
  y = model(x)
  loss = F.cross_entorpy(y, t)
  loss.backward()

  optimizer.step()
```

replaceable

Unified interface to compute preconditioned mini-batch gradient Pg

```
gm = XXXGradientMaker(model, XXXGradientConfig())

dummy_y = gm.setup_model_call(model, x)
gm.setup_loss_call(F.cross_entropy, dummy_y, t)
y, loss = gm.forward_and_backward()
```

equivalent to

```
# PSGD [PsgdGradientMaker]
y = model(x)
loss = F.cross_entropy(y, t)
if step % interval == 0:
  grads = torch.autograd.grad(
            loss, params,
            create_graph=True)
  vs = [torch.randn_like(p)
          for p in params]
  Hvs = torch.autograd.grad(
          grads, params,
          grad_outputs=vs)
  update_preconditioner(vs, Hvs)
else:
  loss.backward()
precondition()
```

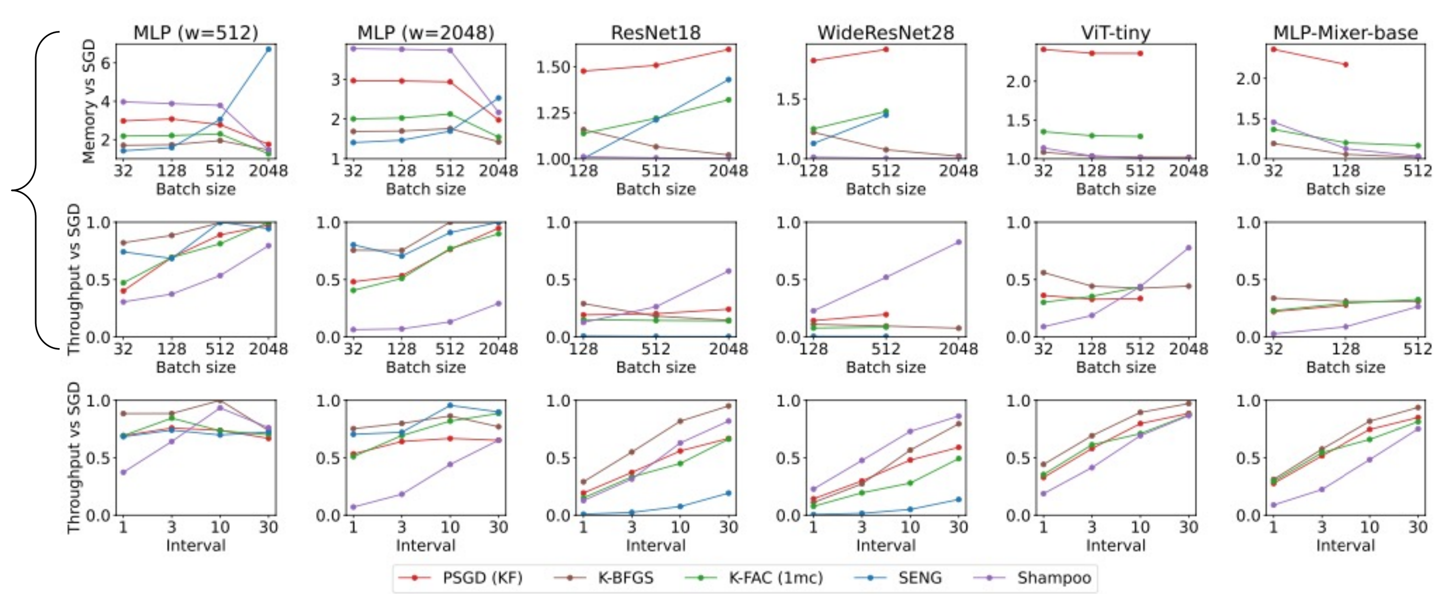
```
# K-FAC (1mc) [KfacGradientMaker]
if step % interval == 0:
  with extend(operations):
    y = model(x)
    loss = F.cross_entropy(y, t)
    p = F.softmax(y)
    log_p = F.log_softmax(y)
    with torch.no_grad():
     t_mc = Categorical(p).sample()
    nll = F.nll_loss(log_p, t_mc)
    nll.backward(retain_graph=True)
  update_preconditioner()
else:
  y = model(x)
  loss = F.cross_entropy(y, t)
loss.backward()
precondition()
```

```
# SENG [SengGradientMaker]
if step % interval == 0:
  with extend(operations):
    y = model(x)
    loss = F.cross_entropy(
            y, t, reduction='sum')
    loss.backward()
    truncate_and_sketch()
    calculate_gram_inv()
    loss /= data_size
else:
  y = model(x)
  loss = F.cross_entropy(
          y, t, reduction='mean')
  loss.backward()
precondition()
```

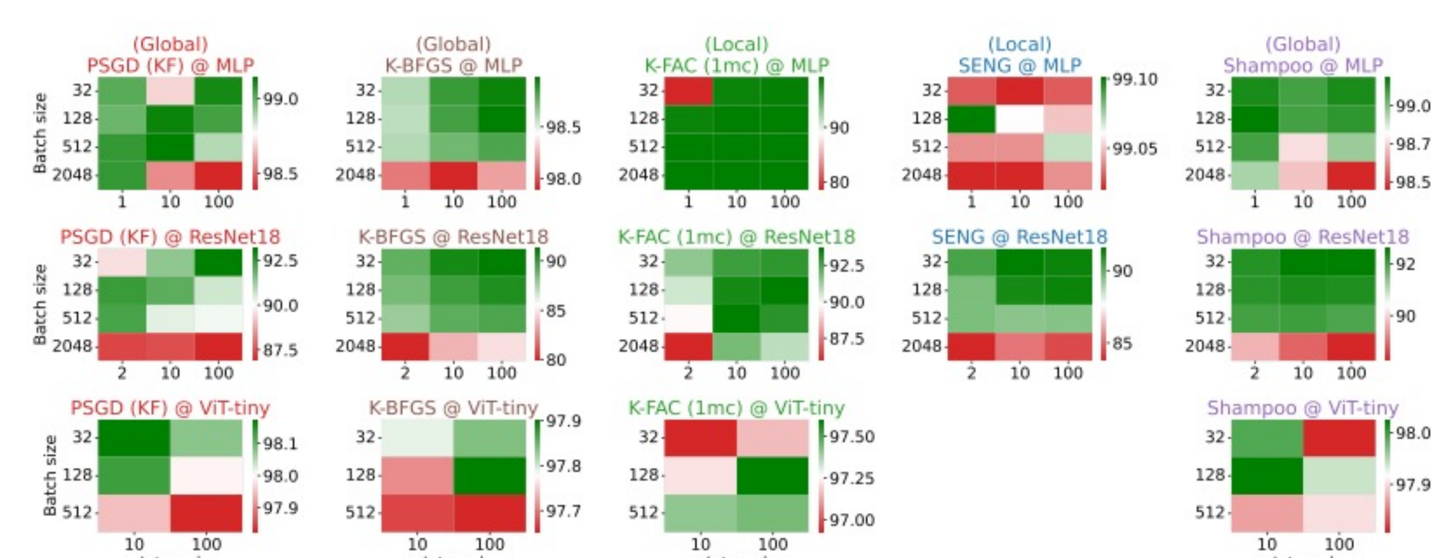
...

Unified interface for gradient preconditioning in PyTorch. XXXGradientMaker ("XXX": algorithm name), offered by ASDL, hides *algorithm-specific* and *complex* operations for Pg in a *unified* way. For training without gradient preconditioning, GradientMaker computes g with the same interface (i.e., no need to switch scripts).

Case Studies with ASDL



The ratio of **peak memory** (>= 1) (top) and **throughput [image/s]** (<= 1) (middle, bottom) of gradient preconditioning methods compared to SGD with various mini-batch sizes B and matrix (C and P) update intervals T, measured on a NVIDIA A100 GPU. For the middle row, T=1. For the bottom row, B=128. Missing points are due to the GPU memory limitation.



Sensitivity of the mini-batch size and matrix update interval to the test accuracy (the best value among different learning rates for each pair is shown). The type of the solver ("Global" or "Local") is indicated at the top of each column. For SENG at ViT-tiny, the plot is not shown because it is not feasible with large mini-batch sizes and only B=32 results are available.

The test accuracy for models achieving the best validation accuracy. For each task, the best accuracy is bolded. "w": width. For ResNet18, the results with 20 and 100 epochs are shown (the number of epochs is fixed for the others). SENG consumes lots of memory and is infeasible with MLP-Mixer-base.

Method	MNIST			CIFAR-10			
	MLP (w=128)	MLP (w=512)	MLP (w=2048)	ResNet18	WideResNet28	ViT-tiny	MLP-Mixer-base
SGD	**98.9**	99.1	**99.2**	91.2 / 95.7	96.7	97.8	97.2
AdamW	98.7	99.0	99.1	89.9 / 94.8	96.0	97.9	**97.7**
PSGD (KF)	**98.9**	99.1	**99.2**	93.3 / **96.2**	96.6	**98.0**	97.5
K-BFGS	98.7	98.9	99.0	91.4 / 95.7	96.5	97.7	97.5
K-FAC (1mc)	98.8	**99.2**	**99.2**	**93.6** / 96.1	**96.9**	97.4	**97.7**
SENG	98.8	99.0	99.1	91.6 / 95.8	96.6	97.7	-
Shampoo	98.8	99.1	**99.2**	92.5 / 96.1	**96.9**	**98.0**	97.4

❖ Key observations

① SENG achieves a high throughput w/ a low memory cost w/ a small mini-batch (and vice versa). For PSGD, K-BFGS, K-FAC, and Shampoo, memory and throughput ratios improve w/ a large mini-batch (Shampoo is particularly slow for most networks otherwise).

② Increasing the matrix update interval significantly improves the throughput, but the degree of speedup depends on methods.

③ "Global" methods (PSGD, K-BFGS, Shampoo) tend to perform better w/ a smaller mini-batch size while a "Local" one (K-FAC) tends to perform better w/ a larger mini-batch size.

④ The best test accuracy for each task is achieved by one of the gradient preconditioning methods, but the best performing method depends on the task.

https://github.com/kazukiosawa/asdl

$$\theta_{t+1} \leftarrow \theta_t - \eta \overbrace{\underbrace{P_t}_{\text{Preconditioning matrix}} \underbrace{g_t}_{\text{Gradient}}}^{\textbf{Preconditioned gradient}}$$

Parameter

Automatic Second-order Differentiation Library
for **Gradient Preconditioning** in Deep Learning

Gradient-based optimization

$$\theta_{t+1} \leftarrow \theta_t - \eta \overbrace{\underbrace{P_t}_{\text{Preconditioning matrix}} \underbrace{g_t}_{\text{Gradient}}}^{\textbf{Preconditioned gradient}}$$

Parameter

- ✓ Supports various gradient preconditioning methods
- ✓ Supports various deep neural networks in PyTorch
- ✓ Easy integration into a PyTorch training script
- ✓ Easy switching of gradient preconditioning methods

Automatic Second-order
Differentiation Library
for Gradient Preconditioning

$$\theta_{t+1} \leftarrow \theta_t - \eta P_t g_t$$

in PyTorch

$$\theta_{t+1} \leftarrow \theta_t - \eta P_t g_t$$

in PyTorch

ASDL

for Gradient Preconditioning

$$\theta_{t+1} \leftarrow \theta_t - \eta P_t g_t$$

in PyTorch

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Author Name, Author Name,
Author Name

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Headline in 34pt should not extend beyond 2-3 lines

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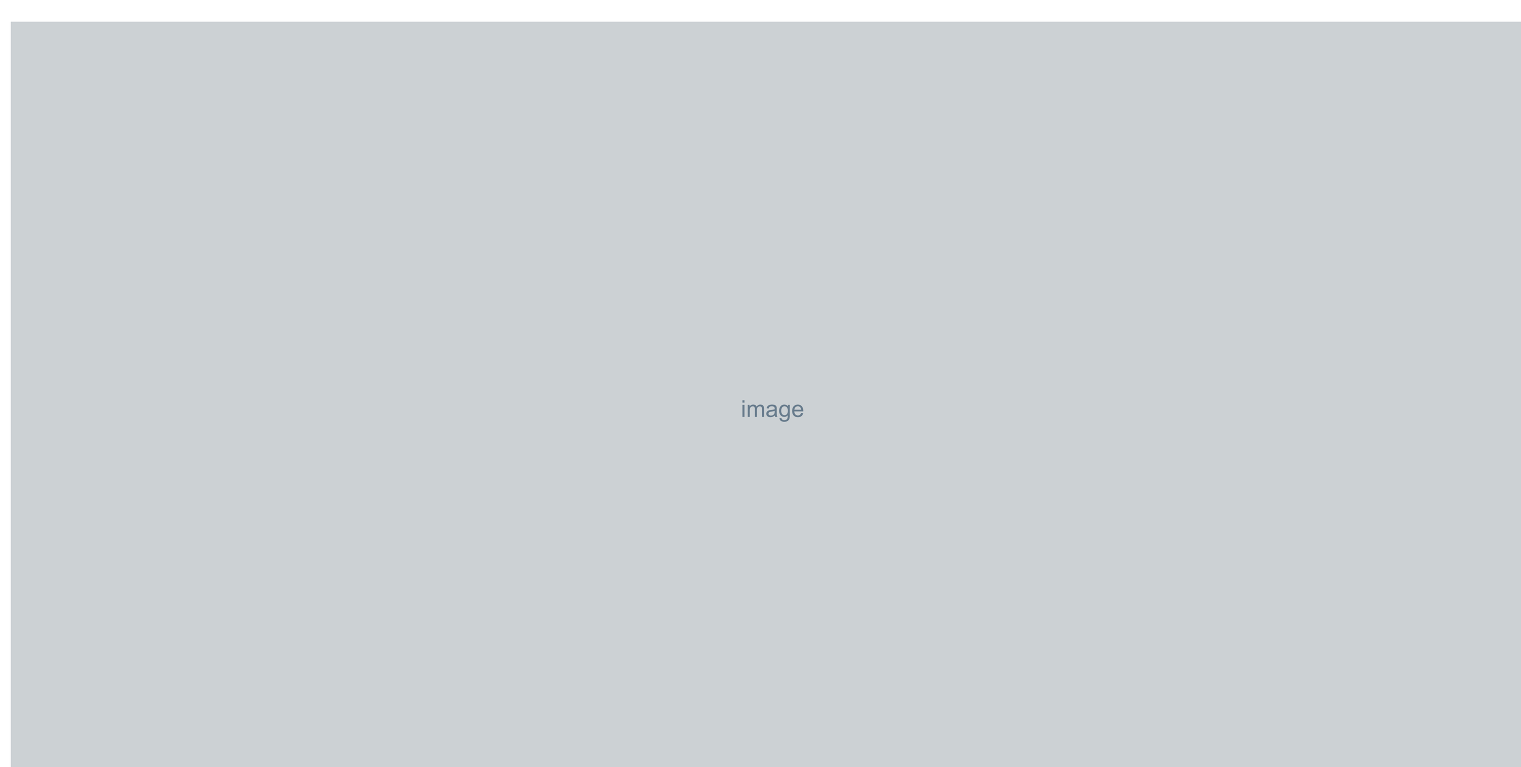

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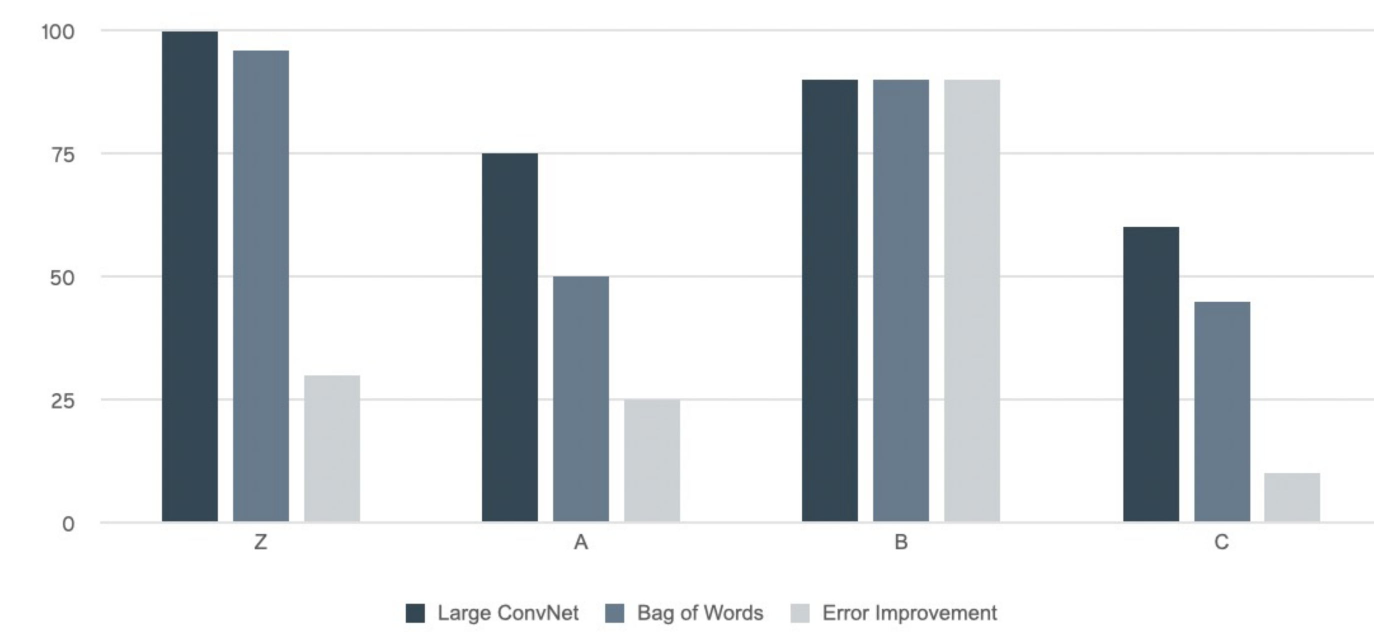

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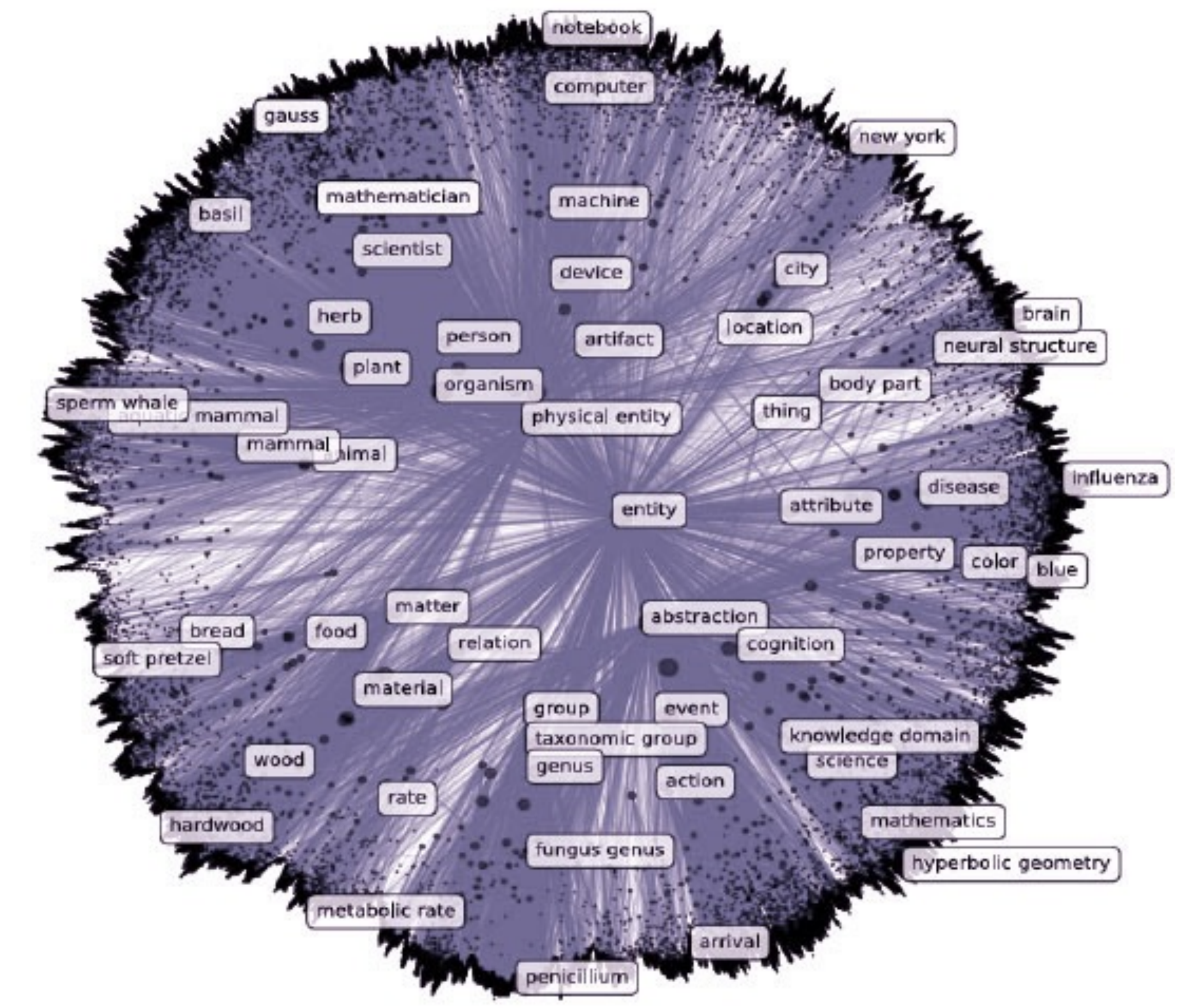
Dimensionality		5	10	20	50
Euclidean	Rank	3542.3	2286.9	1685.9	1281.7
	Map	0.024	0.059	0.087	0.140
Translational	Rank	205.9	179.4	95.3	92.8
	Map	0.517	0.503	0.563	0.566
Poincaré	Rank	4.9	4.02	3.84	3.98
	Map	0.823	0.851	0.855	0.86



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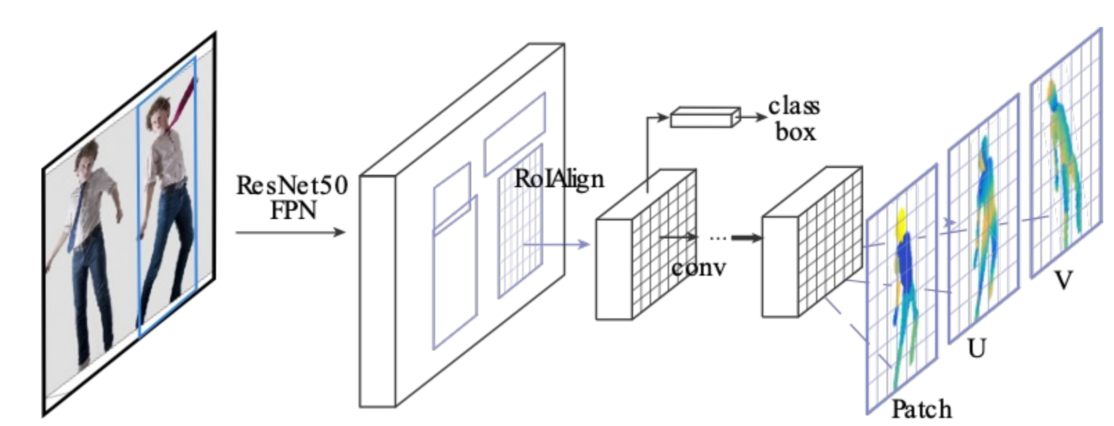

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