# Reinforcement Learning; Uncertainty Quantification & Multitask Learning

YouTube Playlist


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# Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning

YouTube Video

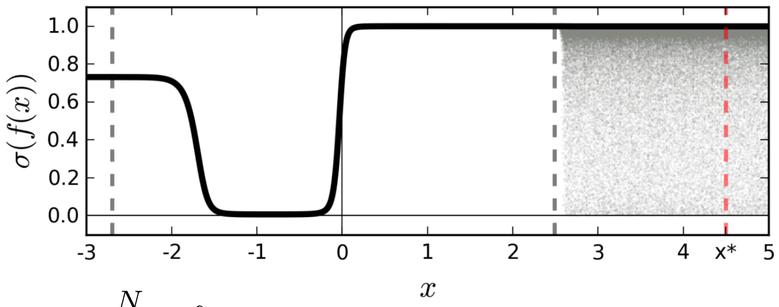
$$p(y|x, W^1, W^2) = \text{softmax}(W^2 \text{ReLU}(W^1 x))$$

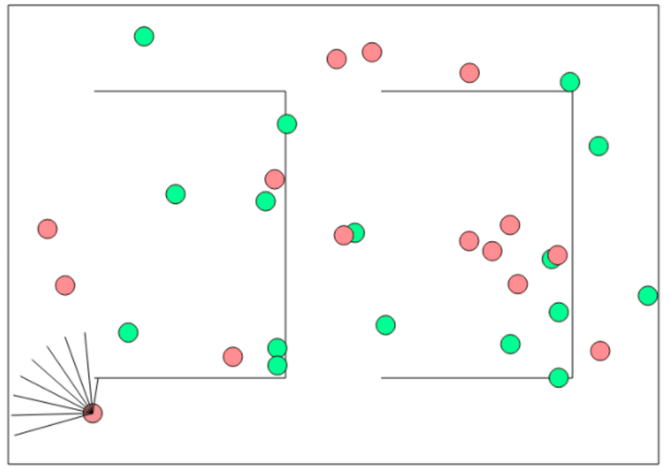
$$x \in \mathbb{R}^{d_0}, W^1 \in \mathbb{R}^{d_1 \times d_0}, W^2 \in \mathbb{R}^{d_2 \times d_1}$$

$$p(W^1) = \mathcal{N}(0, I), p(W^2) = \mathcal{N}(0, I)$$

$$p(y^*|x^*, \mathcal{D}) = \int p(y^*|x^*, W^1, W^2) \underbrace{p(W^1, W^2|\mathcal{D})}_{\text{not tractable}} dW^1 dW^2$$

$\mathcal{D} \rightarrow$ dataset



$$KL[q(W^1, W^2)||p(W^1, W^2|\mathcal{D})] \leq KL[q(W^1, W^2)||p(W^1)p(W^2)] - \sum_{n=1}^{N} \int q(W^1, W^2) \log p(y_n|x_n, W^1, W^2)$$

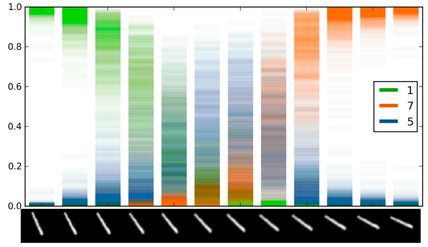
$$q(W^1, W^2) = q(W^1)q(W^2) \rightarrow \text{Variational Distribution}$$

$$q(W^\ell) = p^\ell \mathcal{N}(M^\ell, \sigma^2 I) + (1 - p^\ell)\mathcal{N}(0, \sigma^2 I) \rightarrow \text{Gaussian mixture distribution}$$

$$KL[q(W^\ell)||p(W^\ell)] \approx d^{\ell-1} d^\ell (\sigma^2 - \log(\sigma^2) - 1) + \frac{p^\ell}{2} \|W^\ell\|_2^2 + \text{constant}$$

$$\sigma = 10^{-33} \implies \log(\sigma) = -76$$

$$W^\ell \approx \text{diag}(z^\ell) M^\ell, M^\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}, z^\ell \sim \text{Bernoulli}(p^\ell)$$

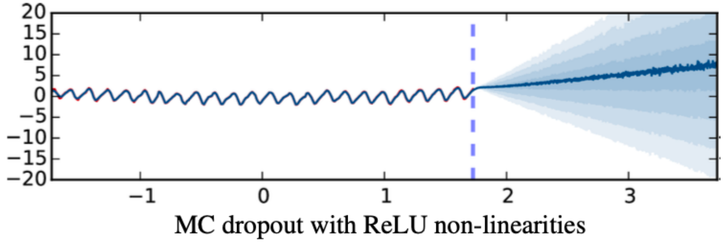


(b) Softmax *output* scatter

$$KL[q(W^1, W^2)||p(W^1, W^2|\mathcal{D})] \leq -\sum_{n=1}^{N} \log p(y_n|x_n, W_n^1, W_n^2) + \frac{p^1}{2} \|M_1\|_2^2 + \frac{p^2}{2} \|M_2\|_2^2$$

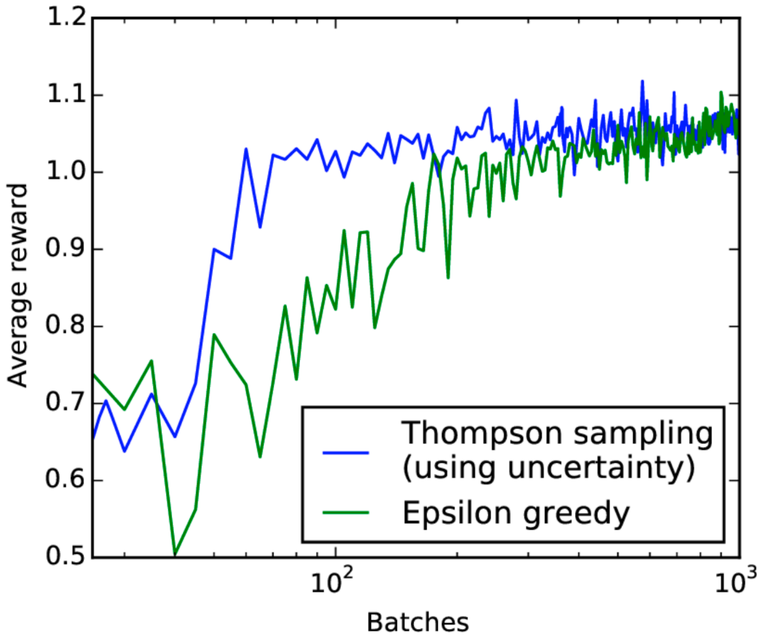
$W_n^\ell \approx \text{diag}(z_n^\ell) M^\ell \rightarrow$ Monte Carlo

Same loss as the one used by dropout!


MC dropout with ReLU non-linearities

$$p(y^*|x^*, \mathcal{D}) \approx \int p(y^*|x^*, W^1, W^2) q(W^1) q(W^2) dW^1 dW^2$$

Use Monte Carlo to obtain the mean and variance of the predictions!




Gal, Yarin, and Zoubin Ghahramani. "Dropout as a bayesian approximation: Representing model uncertainty in deep learning." *international conference on machine learning*. 2016.

# Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles

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$\mathcal{D} = \{x_n, y_n\}_{n=1}^N \rightarrow$ training dataset consisting of $N$ i.i.d data points

$x \in \mathbb{R}^D \rightarrow D$-dimensional features

$y \in \{1, \ldots, K\} \rightarrow$ classification

$y \in \mathbb{R} \rightarrow$ regression

$p_\theta(y|x) \rightarrow$ neural network (probabilistic predictive distribution over labels)

$\theta \rightarrow$ parameters of the neural network

(1) use a proper scoring rule as the training criterion

(2) use adversarial training to smooth the predictive distributions, and

(3) train an ensemble.

$M \rightarrow$ number of neural networks in the ensemble

$\{\theta_m\}_{m=1}^M \rightarrow$ parameters of the ensemble

## Proper Scoring Rules

$S(p_\theta, (y, x)) \rightarrow$ scoring rule (evaluates the quality of the predictive distribution $p_\theta(y|x)$ relative to an event $(y, x) \sim q(y, x)$)

$q(y, x) \rightarrow$ true distribution on $(y, x)$-tuple

$S(p_\theta, q) = \int q(y, \mathbf{x}) S(p_\theta, (y, \mathbf{x})) dy d\mathbf{x} \rightarrow$ expected scoring rule

A proper scoring rule is one where $S(p_\theta, q) \leq S(q, q)$ with equality if and only if $p_\theta(y|x) = q(y|x)$, for all $p_\theta$ and $q$.

$\mathcal{L}(\theta) = -S(p_\theta, q) \rightarrow$ loss

Training using proper scoring rules as training objectives captures ambiguity in targets $y$ for a given $x$.

Cross-entropy loss is a proper scoring rule!

$\mathcal{L}(\theta) = -S(p_\theta, (y, \mathbf{x})) = K^{-1} \sum_{k=1}^K \big(\delta_{k=y} - p_\theta(y = k|\mathbf{x})\big)^2 \rightarrow$ Brier score (also proper)

$$-\log p_\theta(y_n|\mathbf{x}_n) = \frac{\log \sigma_\theta^2(\mathbf{x})}{2} + \frac{\big(y - \mu_\theta(\mathbf{x})\big)^2}{2\sigma_\theta^2(\mathbf{x})} + \text{constant.}$$

regression (also proper)

## Adversarial training to smooth predictive distributions

$\mathbf{x}' = \mathbf{x} + \epsilon \, \text{sign}\big(\nabla_\mathbf{x} \, \ell(\theta, \mathbf{x}, y)\big) \rightarrow$ fast gradient sign method

$(x', y) \rightarrow$ additional training example

## Ensembles: training and prediction

Random initialization of NNs & random shuffling of data

$p(y|\mathbf{x}) = M^{-1} \sum_{m=1}^M p_{\theta_m}(y|\mathbf{x}, \theta_m)$

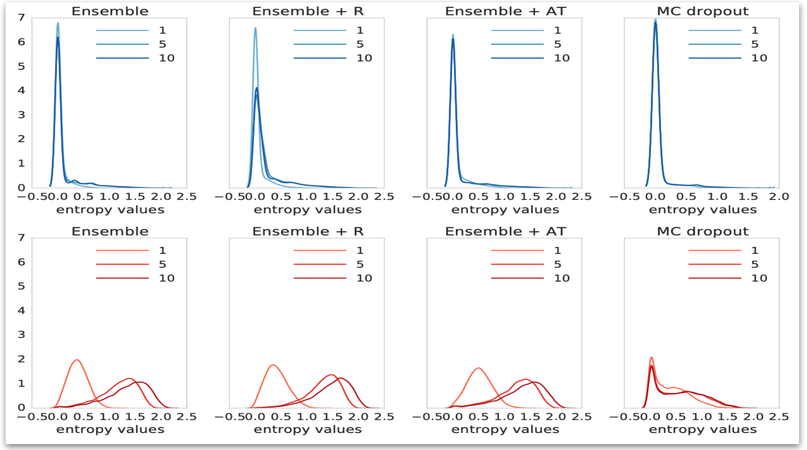
## Evaluation metrics

– negative log likelihood (NLL) – Brier score

– accuracy – root mean squared error (RMSE)

## Domain shift

Higher uncertainty on out-of-distribution examples!




SVHN-CIFAR10

Histogram of the predictive entropy on test examples from known classes (top row) and unknown classes (bottom row), as we vary ensemble size M

Lakshminarayanan, Balaji, Alexander Pritzel, and Charles Blundell. "Simple and scalable predictive uncertainty estimation using deep ensembles." *Advances in neural information processing systems* 30 (2017).

# Model-Agnostic Meta-Learning for Fast Adaptation of Deep Networks

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YouTube Playlist

**Goal:** Train a model on a variety of learning tasks such that it can solve new learning tasks using only a small number of training examples

Tasks as training examples!

$f \rightarrow$ model

$x \longmapsto a$ outputs

observations

episode length

transition distribution

$$\mathcal{T} = \{\mathcal{L}(x_1, a_1, \ldots, x_H, a_H), q(x_1), q(x_{t+1}|x_t, a_t), H\}$$

task

loss function

distribution over initial observations

$H = 1$ in $i.i.d$ supervised problems

$p(\mathcal{T}) \rightarrow$ distribution over tasks

$$\min_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'}) = \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)})$$

Optimize the model parameters such that one or a small number of gradient steps on a new task will produce maximally effective behavior on that task

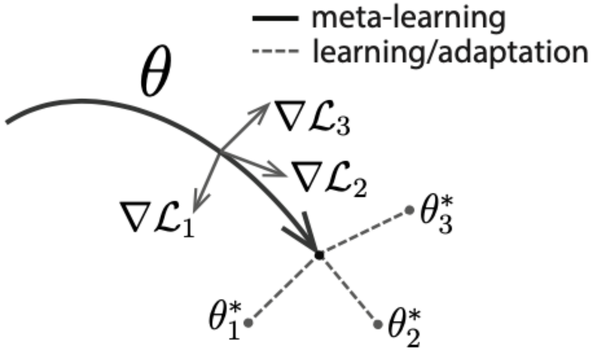
$$\mathcal{L}_{\mathcal{T}_i}(f_\phi) = \sum_{\mathbf{x}^{(j)}, \mathbf{y}^{(j)} \sim \mathcal{T}_i} \|f_\phi(\mathbf{x}^{(j)}) - \mathbf{y}^{(j)}\|_2^2, \rightarrow \text{Regression}$$

$$\mathcal{L}_{\mathcal{T}_i}(f_\phi) = \sum_{\mathbf{x}^{(j)}, \mathbf{y}^{(j)} \sim \mathcal{T}_i} \mathbf{y}^{(j)} \log f_\phi(\mathbf{x}^{(j)}) \rightarrow \text{Classification}$$

$$+ (1 - \mathbf{y}^{(j)}) \log(1 - f_\phi(\mathbf{x}^{(j)}))$$

**Algorithm 1** Model-Agnostic Meta-Learning

**Require:** $p(\mathcal{T})$: distribution over tasks
**Require:** $\alpha$, $\beta$: step size hyperparameters
1: randomly initialize $\theta$
2: **while** not done **do**
3: Sample batch of tasks $\mathcal{T}_i \sim p(\mathcal{T})$
4: **for all** $\mathcal{T}_i$ **do**
5: Evaluate $\nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$ with respect to $K$ examples
6: Compute adapted parameters with gradient descent: $\theta_i' = \theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$
7: **end for**
8: Update $\theta \leftarrow \theta - \beta \nabla_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$
9: **end while**




$$\mathcal{L}_{\mathcal{T}_i}(f_\phi) = -\mathbb{E}_{\mathbf{x}_t, \mathbf{a}_t \sim f_\phi, q_{\mathcal{T}_i}} \left[ \sum_{t=1}^{H} R_i(\mathbf{x}_t, \mathbf{a}_t) \right]$$

**Algorithm 2** MAML for Few-Shot Supervised Learning

**Require:** $p(\mathcal{T})$: distribution over tasks
**Require:** $\alpha$, $\beta$: step size hyperparameters
1: randomly initialize $\theta$
2: **while** not done **do**
3: Sample batch of tasks $\mathcal{T}_i \sim p(\mathcal{T})$
4: **for all** $\mathcal{T}_i$ **do**
5: Sample $K$ datapoints $\mathcal{D} = \{\mathbf{x}^{(j)}, \mathbf{y}^{(j)}\}$ from $\mathcal{T}_i$
6: Evaluate $\nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$ using $\mathcal{D}$ and $\mathcal{L}_{\mathcal{T}_i}$ in Equation (2) or (3)
7: Compute adapted parameters with gradient descent: $\theta_i' = \theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$
8: Sample datapoints $\mathcal{D}_i' = \{\mathbf{x}^{(j)}, \mathbf{y}^{(j)}\}$ from $\mathcal{T}_i$ for the meta-update
9: **end for**
10: Update $\theta \leftarrow \theta - \beta \nabla_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$ using each $\mathcal{D}_i'$ and $\mathcal{L}_{\mathcal{T}_i}$ in Equation 2 or 3
11: **end while**

**Algorithm 3** MAML for Reinforcement Learning

**Require:** $p(\mathcal{T})$: distribution over tasks
**Require:** $\alpha$, $\beta$: step size hyperparameters
1: randomly initialize $\theta$
2: **while** not done **do**
3: Sample batch of tasks $\mathcal{T}_i \sim p(\mathcal{T})$
4: **for all** $\mathcal{T}_i$ **do**
5: Sample $K$ trajectories $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{a}_1, \ldots \mathbf{x}_H)\}$ using $f_\theta$ in $\mathcal{T}_i$
6: Evaluate $\nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$ using $\mathcal{D}$ and $\mathcal{L}_{\mathcal{T}_i}$ in Equation 4
7: Compute adapted parameters with gradient descent: $\theta_i' = \theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$
8: Sample trajectories $\mathcal{D}_i' = \{(\mathbf{x}_1, \mathbf{a}_1, \ldots \mathbf{x}_H)\}$ using $f_{\theta_i'}$ in $\mathcal{T}_i$
9: **end for**
10: Update $\theta \leftarrow \theta - \beta \nabla_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$ using each $\mathcal{D}_i'$ and $\mathcal{L}_{\mathcal{T}_i}$ in Equation 4
11: **end while**


Finn, Chelsea, Pieter Abbeel, and Sergey Levine. "Model-agnostic meta-learning for fast adaptation of deep networks." *arXiv preprint arXiv:1703.03400* (2017).

# Overcoming catastrophic forgetting in neural networks

Continual learning: Learning multiple tasks sequentially

$\theta \rightarrow$ weight and biases of a neural network

$\theta^*_B \rightarrow$ solution to task $B$

$\theta^*_A \rightarrow$ solution to task $A$

Over-parametrization makes it likely that $\theta^*_B$ is close to $\theta^*_A$

Elastic Weight Consolidation (EWC)

$$\mathcal{L}(\theta) = \mathcal{L}_B(\theta) + \frac{1}{2}\lambda \sum_i F_i(\theta_i - \theta^*_{A,i})^2 \rightarrow \text{loss function}$$

Constraining "important" parameters to stay close to their old values!

$p(\theta|\mathcal{D}) \rightarrow$ posterior

$$\log p(\theta|\mathcal{D}) = \underbrace{\log p(\mathcal{D}|\theta)}_{-\mathcal{L}(\theta)} + \log p(\theta) - \log p(\mathcal{D})$$

$\mathcal{D} = \mathcal{D}_A \cup \mathcal{D}_B$

$\mathcal{D}_A \rightarrow$ data on task $A$

$\mathcal{D}_B \rightarrow$ data on task $B$

$$\log p(\theta|\mathcal{D}) = \underbrace{\log p(\mathcal{D}_B|\theta)}_{-\mathcal{L}_B(\theta)} + \underbrace{\log p(\theta|\mathcal{D}_A)}_{\text{interactable}} - \log p(\mathcal{D}_B)$$

Laplace Approximation

$$f(\theta) := \log p(\theta|\mathcal{D}_A) = \underbrace{\log p(\mathcal{D}_A|\theta)}_{-\mathcal{L}_A(\theta)} + \log p(\theta) - \log p(\mathcal{D}_A)$$

$$f(\theta) \approx \underbrace{f(\theta^*_A)}_{\text{const.}} + \underbrace{\nabla_\theta f(\theta^*_A)}_{=0}(\theta - \theta^*_A) + \frac{1}{2}(\theta - \theta^*_A)^T \underbrace{\nabla^2_\theta f(\theta^*_A)}_{\text{Hessian}}(\theta - \theta^*_A)$$

$$\nabla^2_\theta f(\theta^*_A) = -\underbrace{\nabla^2_\theta \mathcal{L}_A(\theta^*_A)}_{\lambda F} + \underbrace{\nabla^2_\theta \log p(\theta)}_{\text{ignore}}$$

$F \rightarrow$ empirical Fisher information matrix

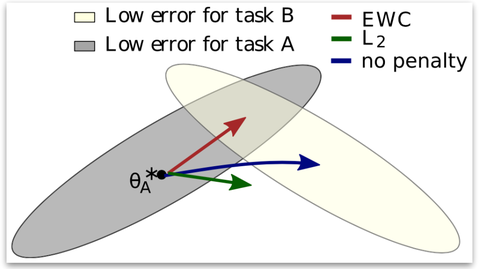
$p(\theta|\mathcal{D}_A) \approx \mathcal{N}(\theta^*_A, \text{diag}(\lambda F)^{-1})$

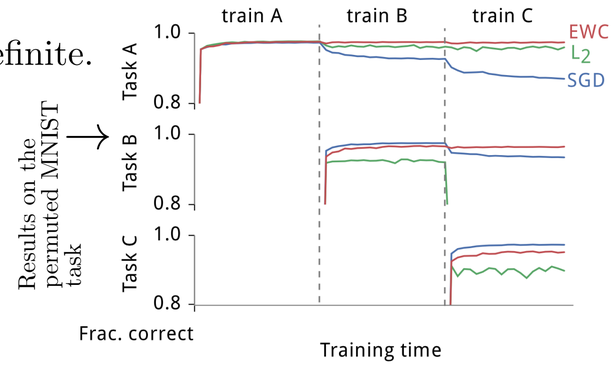
Three key properties of $F$:

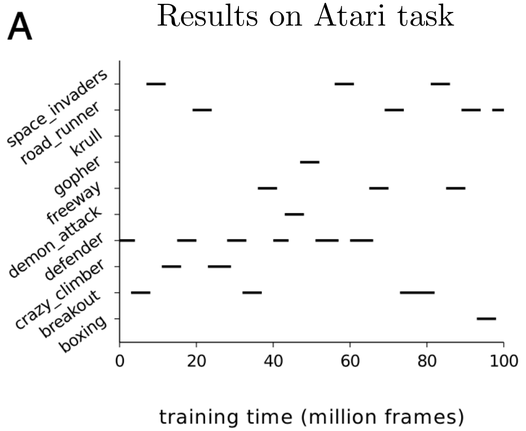
– It is equivalent to the second derivative of the loss near a minimum.

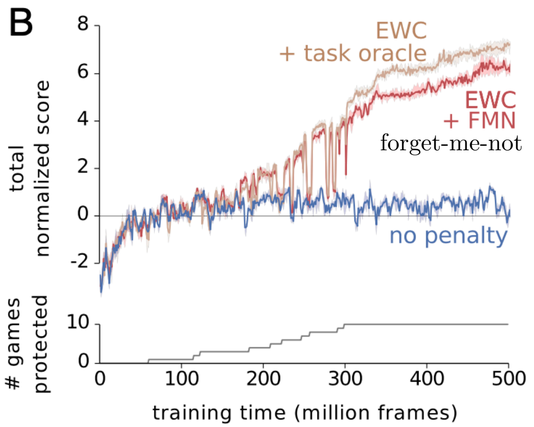
– It can be computed from first-order derivatives alone and is thus easy to calculate even for large models.

– It is guaranteed to be positive semidefinite.




Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *Proceedings of the national academy of sciences* 114.13 (2017): 3521-3526.

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# Questions?

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