Questions for Flat-Minima Optimization of Modern Neural Networks

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Abstract

For training neural networks, flat-minima optimizers that seek to find parameters in neighborhoods having uniformly low loss (flat minima) have been shown to improve upon stochastic and adaptive gradient-based methods. Two methods for finding flat minima stand out: 1. Averaging methods (i.e., Stochastic Weight Averaging, SWA), and 2. Minimax methods (i.e., Sharpness Aware Minimization, SAM). However, despite similar motivations, there has been limited investigation into their properties and no comprehensive comparison between them. In this work, we investigate the loss surfaces from a systematic benchmarking of these approaches across computer vision, natural language processing, and graph learning tasks. This leads us to a hypothesis: since both approaches find flat solutions in orthogonal ways, combining them should improve generalization even further. We verify this improves over either flat-minima approach in 39 out of 42 cases. When it does not, we provide potential explanations. We hope our results across image, graph, and text data will help researchers to improve deep learning optimizers, and practitioners to pinpoint the optimizer for the problem at hand.

1. Introduction

Stochastic gradient descent (SGD) methods are central to neural network optimization (Bottou et al., 2018). Since their initial use, there has been a wealth of research devoted to improving upon it. This includes accelerated gradient / momentum methods (Polyak, 1964; Rumelhart et al., 1988), noise reduction methods (Defazio et al., 2014; Johnson & Zhang, 2013), adaptive gradient methods (Duchi et al., 2010; Zeiler, 2012; Kingma & Ba, 2015), among others. One of the strengths of SGD-based optimizers is their ability to find so-called ‘flat’ minima: large regions that have very similar low loss values (Hochreiter & Schmidhuber, 1997). Theoretical and empirical studies postulate that these regions generalize well, as small shifts between the train and test distributions keep parameters in the flat (low loss) region (Dziugaite & Roy, 2017; Petzka et al., 2021; Chaudhari et al., 2017; Keskar et al., 2017; Jiang et al., 2020). This insight has caused the field of neural network optimization to shift towards developing optimizers that are explicitly designed to find such flat minima.

Flat-minima optimizers largely fall into two popular approaches: 1. Averaging methods (Polyak & Juditsky, 1992), and 2. Minimax methods (Foret et al., 2021). Averaging methods are based on the intuition that, near a minimum, flatness causes an optimizer to slow down, leaving many iterates in or around that flat region. Therefore, averaging iterates near the end of optimization will produce a solution that is pulled towards these flatter regions (see Figure 1, left)). On the other hand, minimax methods minimize the maximum loss around a neighborhood of the current iterate. This way, a region around the iterate is designed to have uniformly low loss (see Figure 1, right). These approaches have shown impressive gains over prior work. For example, flat-minima optimization can lead to similar performance gains as advanced data augmentation techniques (Chen et al., 2021), avoiding the domain expertise required to design careful data transformations that preserve label semantics.

However, even though both approaches have the same goal,
we are unaware of a systematic comparison between them. As such, it is tricky for researchers to improve upon these approaches and for practitioners to know which approach is best for the problem at hand.

Here we fill in this missing piece by benchmarking a representative method for averaging, Stochastic Weight Averaging (SWA) (Izmailov et al., 2018), and for minimax optimization, Sharpness-Aware Minimization (SAM) (Foret et al., 2021). We select these due to their scalability to large models and excellent results across a variety of learning tasks (Nikishin et al., 2018; Athiwaratkun et al., 2019; Chen et al., 2021a; Bahri et al., 2021). This large-scale experimental study compares them across different domains (computer vision, natural language processing, graph learning), model types (multi-layer perceptrons, convolutional networks (Le-Cun et al., 1989), transformers (Vaswani et al., 2017)) and learning environments (classification, self-supervised learning, open-domain question answering, natural language understanding, and node/graph/link property prediction).

We analyze the loss and accuracy around and between solutions of each flat-minima approach on two prototypical settings. We find that each approach finds flat solutions in complementary ways. Better, we observe that it is possible to find flatter regions around minimax solutions, and that these regions correspond to increased accuracy. This leads us to a hypothesis: combining both approaches, a method we refer to as weight-averaged sharpness-aware minimization (WASAM), should further drive down generalization error. We test this hypothesis and the results confirm this: on average, taking the moving average of minimax solutions improves accuracy. In 39 out of 42 cases, WASAM performs at least as well as the worst flat-minima optimizer. When flat-minima optimizers do not help, we investigate the loss/accuracy surfaces and notice different properties compared to cases where they do (e.g., clear discrepancies between the shapes of loss and accuracy curves). To conclude, we summarize the results, and list four limitations that motivate future work directions.

2. Background and Related Work

2.1. Stochastic Gradient Descent (SGD)

The classic optimization framework of machine learning is empirical risk minimization

$$
L(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(x_i; \theta)
$$

where $\theta \in \mathbb{R}^d$ is a vector of parameters, $\{x_1, \ldots, x_N\}$ is a training set of inputs $x_n \in \mathbb{R}^D$, and $\ell(x; \theta)$ is a loss function quantifying the performance of parameters $\theta$ on $x$. SGD samples a minibatch $S \subset \{1, \ldots, N\}$ of size $|S| \ll N$ from the training set and computes the gradient

$$
\nabla L(\theta) = \frac{1}{|S|} \sum_{i \in S} \nabla \ell(x_i; \theta).
$$

The parameters get updated following this gradient

$$
\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t),
$$

for a length specified by $\eta$, the learning rate. Previous research has established that this vanilla SGD training often falls into sharp minima of the loss surface (Chaudhari et al., 2017; Wang et al., 2021), in particular when the batch size $|B|$ is large (Keskar et al., 2017). Most of the research improving SGD for neural networks has been devoted to reducing its sensitivity to $\eta$ (Zeiler, 2012; Duchi et al., 2010; Kingma & Ba, 2015) or handling the noise introduced by minibatch sampling (Defazio et al., 2014; Johnson & Zhang, 2013). Recently, work has shifted to design optimization methods that explicitly find flat minima, often using one of two approaches: averaging or minimax optimization.

2.2. Averaging: Stochastic Weight Averaging (SWA)

The idea of averaging SGD iterates dates back to Polyak & Juditsky (1992), who proved the highest possible rates of convergence for a variety of classical optimization problems. SWA is a modern take on this idea, with the motivation being the following observation about SGD’s behavior when training neural networks: it often traverses regions of the weight space that correspond to high-performing models, but rarely reaches the central points of this optimal set. Averaging the parameter values over iterations moves the solution closer to the centroid of this space of points.

The SWA update rule is the cumulative moving average

$$
\theta^{\text{SWA}}_{t+1} = \theta^{\text{SWA}}_t + \frac{\theta^\text{SGD}_t}{k + 1},
$$

where $k$ is the number of distinct parameters averaged so far and $t$ is the SGD iteration number.\footnote{SWA parameters are constant between averaging steps.}

SWA has two hyper-parameters: the update frequency $\nu$ and starting epoch $E$. When using a constant learning rate, Izmailov et al. (2018) suggests to update the parameters once after each epoch, i.e. $\nu \approx \frac{N}{T}$, and starting at $E \approx 0.75T$, where $T$ is the training budget required to train the model until convergence with conventional SGD training. SWA’s computational overhead consists of the memory requirement for an additional copy of the model weights ($\theta^{\text{SWA}}$).

The reason for starting SWA near the end of training is that this is when SGD will most likely encounter high-performing models. He et al. (2019) postulate that SWA is effective, because most neural network loss surfaces have
asymmetric sides, and SWA biases the solution towards the flatter sides (Figure 1, left).

**Related Work (SWA)** An alternative model weight averaging strategy is exponential moving averaging, which has been employed in deep reinforcement learning (Lillicrap et al., 2016), semi-supervised settings (Tarvainen & Valpola, 2017), or image models (Wightman, 2019). Athiwaratkun et al. (2019) propose to train consistency-based methods with SWA. Maddox et al. (2019) approximate the posterior distribution over neural network weights by parameterizing a Gaussian distribution with the SWA solution as the first moment. Nikishin et al. (2018) show that SWA can improve stability in deep reinforcement learning. Cha et al. (2021) introduce a SWA variant for domain generalization tasks.

### 2.3. Minimax: Sharpness-Aware Minimization (SAM)

While SWA is implicitly biased towards flat minima, SAM explicitly approximates the flatness around parameters \( \theta \) to guide the parameter update. It first computes the worst-case perturbation \( \epsilon \) that maximizes the loss within a given neighborhood \( \rho \), and then minimizes the loss w.r.t. the perturbed weights \( \theta + \epsilon \).

Formally, SAM finds \( \theta \) by solving the minimax problem:

\[
\min_{\theta} \max_{\|\epsilon\|_2 \leq \rho} L(\theta + \epsilon),
\]

where \( \rho \geq 0 \) is a hyperparameter.

To find the worst-case perturbation \( \epsilon^* \) efficiently in practice, Foret et al. (2021) approximates eq. (5) via a first-order Taylor expansion of \( L(\theta + \epsilon) \) w.r.t. \( \epsilon \) around \( \theta \), obtaining

\[
\epsilon^* \approx \arg \max_{\|\epsilon\|_2 \leq \rho} \epsilon^T \nabla_\theta L(\theta) \approx \rho \frac{\nabla_\theta L(\theta)}{\nabla_\theta L(\theta)}.
\]

In words, \( \epsilon^* \) is simply the scaled gradient of the loss function w.r.t. to the current parameters \( \theta \). Given \( \epsilon^* \), the altered gradient used to update the current \( \theta_t \) (in place of \( g(\theta_t) \)) is

\[
\nabla_\theta \max_{\|\epsilon\|_2 \leq \rho} L(\theta + \epsilon) \approx \epsilon^* \frac{\nabla_\theta L(\theta)}{\nabla_\theta L(\theta)}.
\]

Due to eq. (6), SAM’s computational overhead consists of an additional forward and backward pass per parameter update step compared to the base optimizer.

**Related Work (SAM)** Concurrently to Foret et al. (2021), Wu et al. (2020) propose an almost identical minimax objective, additionally including perturbations of the training data, and layer-dependent scaling of \( \rho \). Kwon et al. (2021) propose to adaptively scale the size of the neighborhood \( \rho \) in relation to the model parameter’s norm to avoid sensitivity to parameter re-scaling. Du et al. (2021) aim at reducing SAM’s computational cost by proposing two approximation strategies. Brock et al. (2021) propose to ameliorate the additional cost of eq. (6) by only employing 20% of the mini-batch to compute the gradients necessary for \( \epsilon \). Chen et al. (2021a) show that SAM is effective on Vision Transformers (ViTs) and MLP-Mixer architectures, which are more prone to land in sharp minima than ones that include convolutional layers. Bahri et al. (2021) demonstrates that SAM can improve the generalization of text-to-text transformer (T5) language models for natural language understanding and question-answering tasks.

### 2.4. Comparing Neural Network Minima

In this work, we aim to compare the trained models produced by the respective flat-minima optimizer, i.e. the solutions or minima found by the optimization procedure. One popular way to compare any two networks is to investigate the behavior of the loss landscape along the line between them. Previous studies successfully used such linear interpolations to gain insights and develop new methods, e.g., for training dynamics (Goodfellow & Vinyals, 2015; Frankle, 2020; Fort et al., 2020; Lucas et al., 2021; Yang et al., 2021), regularization (Li et al., 2018; Geiping et al., 2021), network pruning (Frankle et al., 2020), transfer learning (Neyshabur et al., 2020), or multitask learning (Mirzadeh et al., 2021).

If there exists no high-loss barrier between two networks along the linear interpolation, we call them (linearly) mode-connected or say that their solutions are located in the same basin (or valley) (Garipov et al., 2018b). Neyshabur et al. (2020) formally define the notion of two solutions being in the same basin. Informally, a basin is an area in the parameter space where the loss function has relatively low values. Due to the non-linear and compositional structure of neural networks, the linear combination of the weights of two accurate models does not necessarily define an accurate model. Hence, we generally expect high-loss barriers along the linear interpolation path.

While there are alternative distance measures that could be used to compare two networks, they typically either (a) do not offer clear interpretations, as pointed out by Frankle et al. (2020), or (b) yield trivial network connectivity results, such as non-linear low-loss paths, which can be found for any two network minimizers (Draxler et al., 2018; Garipov et al., 2018a; Gotmare et al., 2019; Fort & Jastrzebski, 2019).

To the best of our knowledge, prior analysis of flat-minima optimizers has only focused on verifying that they indeed find flatter solutions than non-flat methods through sharpness measures based on the Hessian matrix of the loss function.

\^{3}We refer to optimizers not intentionally designed to find flat regions as non-flat, although it is not guaranteed they are sharper.
tion (Chaudhari et al., 2017; Petzka et al., 2021), loss landscape visualizations generated by normally distributed direction vectors (Izmailov et al., 2018; Chen et al., 2021a) or Monte-Carlo approximations of the minimizer’s neighborhood (Foret et al., 2021; Cha et al., 2021). Instead, here we compare the surfaces of flat minima obtained by different optimizers.

3. Surfaces of Flat Minima

In this section, we investigate the loss and accuracy near the solutions of the flat-minima optimizers to better understand their qualitative differences. For two tasks where these optimizers improve over the baseline, we begin by investigating interpolations between non-flat solutions and both averaging and minimax solutions (Section 3.1). Then, we look closer at the loss/accuracy surfaces in other directions around flat solutions (Section 3.2). This lead us to our hypothesis: **SWA and SAM work in complementary ways that can be combined to improve generalization.** We end by investigating cases where flat-minima optimizers do not improve over non-flat solutions (Section 3.3).

We choose the following two disparate learning settings for analyzing flat-minima optimizers: (i) a well-known image classification task, widely used for evaluation in flat-minima optimizer papers, and (ii) a novel, challenging Python code summarization task, on which state-of-the-art models achieve only around 16% F1 score, and that has not been explored yet in the flat-minima literature. Specifically, for (i), we investigate the loss/accuracy surfaces of a WideResNet28-10 (Zagoruyko & Komodakis, 2016) model on CIFAR-100 (Krizhevsky, 2009) (baseline non-flat optimizer: SGD with momentum (SGD-M)) (Rumelhart et al., 1988). For (ii), we use the theoretically-grounded Graph Isomorphism Network (Xu et al., 2019) model on OGB-Code2 (Hu et al., 2020) (baseline optimizer: Adam (Kingma & Ba, 2015)). All optimizers start from the same initialization. We denote the minimizer produced by the non-flat methods (SGD-M and Adam) by $\theta^{\text{NF}}$ and the flat ones by $\theta^{\text{SWA}}$ and $\theta^{\text{SAM}}$. Please see Appendix A for details on the visualizations.

### 3.1. What is between non-flat and flat solutions?

We start by comparing the similarity of flat and non-flat minimizers through linear interpolations. This analysis allows us to understand if they are in the same basin, and how close they are to a region of sharply-increasing loss, where we expect loss/accuracy to differ widely between train and test.

Our first observation is that Figures 2a and 2e show that for both tasks, $\theta^{\text{SWA}}$ (marker: +) is in the same basin as $\theta^{\text{NF}}$ (marker: •). Additionally, when going in the direction from $\theta^{\text{SWA}}$ to $\theta^{\text{NF}}$ (i.e., $\alpha > 1$), $\theta^{\text{NF}}$ is near the periphery of a sharp increase in loss. Conversely, $\theta^{\text{SWA}}$ finds flat regions that change very slowly in loss. This finding confirms and extends those of He et al. (2019) to models beyond ResNet and PreResNet, and datasets outside of CIFAR100.

The bias of SWA to flatter loss beneficially transfers to the accuracy landscape too: Figures 2b and 2f show the accuracy/F1 score rapidly dropping off approaching and beyond $\theta^{\text{NF}}$. Interestingly, in Figures 2e and 2f, we see that for OGB-Code2, for $\alpha < 0$, there exist solutions with even better training loss/accuracy but worse test loss/accuracy. However, $\theta^{\text{SWA}}$ is very close to the test accuracy maximizer along this interpolation (we will see in Section 5 that $\theta^{\text{SWA}}$ consistently improves over $\theta^{\text{NF}}$).

Turning now to SAM, $\theta^{\text{SAM}}$ (marker: ×) and $\theta^{\text{NF}}$ are not in the same basin: Figures 2c and 2g show that there is a significant loss barrier between them, respectively. This is an interesting result because we expect different basins to
produce qualitatively different predictions, one of the motivations behind combining models via ensembling (Huang et al., 2017; Lakshminarayanan et al., 2017). Figures 2d and 2h show that $\theta^{\text{SAM}}$ and even nearby points in parameter space achieve higher accuracies/F1 scores (i.e. generalize better) than $\theta^{\text{NF}}$ and points around it. We investigate the $\theta^{\text{SAM}}$ basin further in Section 3.2.

Lastly, another surprise is that Figure 2g shows $\theta^{\text{SAM}}$ being located in a sharp training loss minimum whose loss is much higher than $\theta^{\text{NF}}$. Yet, its test loss is only slightly higher. On the other hand, Figure 2h shows that $\theta^{\text{SAM}}$ generalizes better w.r.t. the F1 score (the metric of interest for OGB-Code2). We give an explanation for this in the next section.

### 3.2. What is around flat solutions?

The linear interpolations in the previous section are instructive for differentiating flat minimization approaches. Now, we are interested in understanding if it is possible to further improve solutions by investigating them independently. Specifically, because each NN model is a point in such a high-dimensional space, the loss/accuracy surface can look completely unfamiliar when starting from these same solutions, but moving in different directions. Here, we investigate these different directions. Starting from the same solutions as described in the previous section, we show the planes defined by two Gaussian random vectors pointing away from them. We plot the solutions of SWA (●) and SAM (×), as well as the test accuracy/F1 maximizer in the plane (■) in Figure 3.

We first observe that around the SWA solutions shown in Figures 3a and 3b (WideResNet28-10/CIFAR100) the location of the highest test accuracy is far away from the SWA solution. Further, it does not correspond to a particularly flat region of training loss, or have other notable properties.

Similarly, around the SWA solutions shown in Figures 3e and 3f (GIN/OGB-Code2) the highest test F1 score point, while close to SWA, is also hard to identify: there are flatter regions (in training loss) but that correspond to worse test accuracy. It seems difficult to use the training data to improve generalization over the SWA solution (of course this is not exhaustive evidence, as we only consider two random directions in a high-dimensional space).

For SAM, the first observation is that we have a better explanation for why the losses of $\theta^{\text{SAM}}$ are surprisingly high in Figure 2g: it finds a saddle point which is very near the maximizer of test F1, shown in Figures 3g and 3h. Additionally, around the SAM solutions, the test accuracy/F1 maximizers appear closer, and seem to better correspond to flatter training loss regions. In Figures 3c and 3d, in all directions from the highest test accuracy point, the training loss increases slowly. In Figures 3g and 3h the highest test loss is right between the train loss maximizer and minimizer that make up the saddle point. This provides evidence that it may be possible to use these training signals to find flatter regions around SAM solutions, which correspond to higher test accuracy/F1.

### 3.3. When do flat-minima optimizers fail?

Here, we audit one of the cases (3 out of 42 cases, as we will later see in Section 5), where $\theta^{\text{SWA}}$ and $\theta^{\text{SAM}}$ do not improve over $\theta^{\text{NF}}$: training a GraphSAGE (Hamilton et al., 2017) model on OGB-Proteins: a protein-protein interaction graph where the goal is to predict the presence of protein functions (multi-label binary classification) (Hu et al., 2020). $\theta^{\text{SWA}}$ performs noticeably worse; $\theta^{\text{SAM}}$ performs about equally well.

Figure 4 shows two linear interpolations: between $\theta^{\text{NF}}$ (ADAM) and (1) $\theta^{\text{SWA}}$ (Figures 4a and 4b), and (2) $\theta^{\text{SAM}}$...
(Figures 4c and 4d). In contrast to success cases in Figure 2, here: (a) for both SWA and SAM, the training loss minimizer is very uncorrelated with the test loss minimizer; (b) SAM and ADAM seem to be in the same test loss/accuracy basin. Investigating the causes of these we argue is a useful direction for future work.

Figure 4. GraphSAGE on OGB-Proteins: Adam’s (●) solution performs about equally well as SAM (×), and better than SWA (+).

Figure 5. Training (blue) / test (red) losses (—) / accuracies (…) between non-flat baseline (●) ↔ SWA (+), SAM (×) ↔ WASAM (★).

4. Weight-Averaged SAM

In the previous section, we made three key observations: 1. SWA and SAM find different basins; 2. SWA can find flatter regions around the baseline optimizer it is averaging; 3. There exist flatter regions around SAM solutions that correspond to higher accuracy. These lead us to a hypothesis: applying the averaging technique of SWA to SAM iterates should further improve generalization. We refer to this technique as weight-averaged sharpness-aware minimization. Algorithm 1 describes the procedure in more detail.

Algorithm 1 WASAM

**Input:** Loss function $L$, training budget in number of iterations $b$, training dataset $\mathcal{D} := \bigcup_{t=1}^n \{x_t\}$, mini-batch size $|\mathcal{B}|$, neighborhood radius $r$, averaging start epoch $E$, averaging frequency $\nu$, (scheduled) learning rate $\eta$, initial weights $\theta_0$.

**for** $k \leftarrow 1, \ldots, b$ **do**

Sample a mini-batch $\mathcal{B}$ from $\mathcal{D}$

Compute worst-case perturbation $\tilde{e} \leftarrow r \frac{\nabla L(\theta)}{\|\nabla L(\theta)\|_2}$

Compute gradient $g \leftarrow \nabla L(\theta + \tilde{e})$

Update parameters $\theta_{i+1} \leftarrow \theta_i - \eta g$

if $k \geq E$ and $\text{mod}(k, \nu) = 0$ then

\[ \theta_{i+1}^{\text{WASAM}} = (\theta_{i+1}^{\text{WASAM}} \cdot n + \theta_{i+1}) / (n + 1) \]

**end if**

**end for**

return $\theta^{\text{WASAM}}$

Starting with the first of the two previously analyzed settings (WideResNet28-10/CIFAR100), Figures 5a, and 5b show that $\theta^{\text{WASAM}}$ (marker: ⋄) achieves the lowest test loss and highest test accuracy, respectively. What stands out in comparison to the previous plots is $\theta^{\text{SAM}}$’s (×) proximity to sharp sides, surprisingly similar to $\theta^{\text{SF}}$ (●) here and in Figures 2c and 2e.

In GIN/OGB-Code2, one unanticipated finding is that $\theta^{\text{WASAM}}$ escapes the saddle point of $\theta^{\text{SAM}}$ that we found in 3g (appearing here as a maximum), as shown in Figure 5c. This is likely because SAM traversed nearby flatter regions before arriving at the saddle point. In terms of F1 score, Figure 5d shows that while $\theta^{\text{SWA}}$ (+) and $\theta^{\text{SAM}}$ perform about equally well, the flatter region found by $\theta^{\text{WASAM}}$ improves over both.

In the same two settings we previously investigated, WASAM does not just perform as well as the best of SWA or SAM, but because of their complementary approaches to finding flatness, the combination outperforms both.

5. Benchmark Results

We compare flat minimizers SWA, SAM, and WASAM over the baseline non-flat minimizers across a range of different
tasks in the domains of computer vision, natural language processing, and graph representation learning. All results have been averaged at least three times across random seeds and we report the corresponding standard error. We bold the best-performing approach and any approach whose average performance plus standard error overlaps it.

**Hyper-parameters.** For all architectures and datasets, we set hyperparameters shared by all methods (e.g., learning rate) mostly to values cited in prior work; sometimes with minor modifications, e.g., adjusting the batch size to be compatible with our GPUs’ memory capacities. For flat-minima optimizers we select hyper-parameters using a grid search over a held out validation set. Specifically, for SWA we follow Izmailov et al. (2018) and hold the update frequency \( \nu \) constant to once per epoch and tune the start time \( E \in \{0.5T, 0.6T, 0.75T, 0.9T\} \) (\( T \) is the number of baseline training epochs). Izmailov et al. (2018) argue that in order to encourage exploration of the basin, a cyclical learning rate starting from \( E \) can help. For the sake of simplicity, we average the iterates of the baseline directly, but include even earlier training times (i.e., \( 0.5T, 0.6T \)). For SAM, we tune its neighborhood size \( \rho \in \{0.01, 0.02, 0.05, 0.1, 0.2\} \), similarly to previous work (Foret et al., 2021; Bahri et al., 2021).

Please see Appendix B for the values of all hyper-parameters and additional training details.

### 5.1. Computer Vision

**Supervised Classification (SC).** We evaluate the CNN architectures WideResNets (Zagoruyko & Komodakis, 2016) with 28 layers and width 10, and PyramidNet (PN) with 110 layers and widening factor 272 (Han et al., 2017) as well as Vision Transformer (ViT) (Dosovitskiy et al., 2021) and MLP-Mixer (Tolstikhin et al., 2021) on CIFAR10, CIFAR100, ImageNet16, and ImageNet16-120 datasets (Hu et al., 2020). The tasks are node property pre-selections: horizontal flip, padding by four pixels, random crop, and cutout (Devries & Taylor, 2017).

**Self-Supervised Learning (SSL).** We consider the following methods on CIFAR10 and ImageNet16:

| Task | Model | Baseline | SWA | SAM | WASAM |
|------|-------|----------|-----|-----|-------|
| SC: CIFAR10 | WRN-28-10 | 96.78\pm0.03 | −0.09\pm0.01 | +0.34\pm0.00 | +0.25\pm0.05 |
| | PN-272 | 96.73\pm0.14 | +0.22\pm0.14 | +0.42\pm0.06 | +0.41\pm0.02 |
| | ViT-B-16 | 98.95\pm0.02 | −0.04\pm0.01 | +0.07\pm0.01 | +0.10\pm0.01 |
| | Mixer-B-16 | 96.69\pm0.03 | +0.03\pm0.01 | +0.19\pm0.06 | +0.22\pm0.06 |
| SC: CIFAR100 | WRN-28-10 | 80.93\pm0.15 | +1.02\pm0.06 | +1.82\pm0.14 | +2.24\pm0.14 |
| | PN-272 | 80.86\pm0.12 | +1.85\pm0.04 | +2.33\pm0.06 | +2.69\pm0.00 |
| | ViT-B-16 | 92.77\pm0.07 | −0.12\pm0.05 | +0.19\pm0.00 | +0.13\pm0.07 |
| | Mixer-B-16 | 83.73\pm0.08 | +0.43\pm0.05 | +0.52\pm0.02 | +0.97\pm0.12 |
| SSL: CIFAR10 | MoCo | 89.25\pm0.07 | −0.03\pm0.10 | −0.25\pm0.06 | −0.17\pm0.10 |
| | SimCLR | 88.66\pm0.08 | −0.07\pm0.06 | +0.05\pm0.04 | −0.13\pm0.06 |
| | SimSiam | 89.12\pm0.22 | +0.12\pm0.26 | +0.07\pm0.10 | +0.11\pm0.16 |
| | BarlowTwins | 86.34\pm0.26 | −0.09\pm0.19 | +0.09\pm0.15 | +0.14\pm0.05 |
| | BYOL | 90.32\pm0.14 | +0.70\pm0.05 | +0.14\pm0.03 | +0.21\pm0.07 |
| | SwaV | 87.25\pm0.07 | +0.09\pm0.06 | +0.07\pm0.12 | +0.02\pm0.06 |
| SSL: ImageNet | MoCo | 81.74\pm0.14 | +0.97\pm0.12 | +0.91\pm0.32 | +1.40\pm0.10 |
| | SimCLR | 83.29\pm0.22 | +0.95\pm0.25 | +0.18\pm0.24 | +1.07\pm0.13 |
| | SimSiam | 81.77\pm0.14 | +0.20\pm0.37 | +0.33\pm0.28 | +0.18\pm0.26 |
| | BarlowTwins | 77.49\pm0.31 | +0.20\pm0.16 | +0.47\pm0.27 | +0.66\pm0.57 |
| | BYOL | 84.16\pm0.14 | +0.76\pm0.08 | +0.15\pm0.25 | +0.31\pm0.13 |
| | SwaV | 88.16\pm0.31 | +1.04\pm0.27 | +0.03\pm0.10 | +1.03\pm0.09 |

Table 1. CV test results: Supervised Classification (SC), and Self-Supervised Learning (SSL) tasks.

We observe that flat minimizers nearly always improve test accuracies for image classifications and WASAM is the best performing method in all but one case. In semi-supervised learning on CIFAR-10, the baseline non-flat optimizer is nearly always the best and the highest performing model is BYOL optimized with SWA. Whereas for ImageNet, WASAM is again the best in all but one case.

### 5.2. Natural Language Processing

We first consider the task of open domain question answering (ODQA) using a T5-based generative model Fusion-In-Decoder (FiD) (Izacard & Grave, 2021). We evaluate the FiD-base on the datasets of Natural Questions (NQ) (Kwiatkowski et al., 2019) and TriviaQA (Joshi et al., 2017). We also consider a range of natural language understanding tasks included in the GLUE benchmark (Wang et al., 2018), which cover acceptability, sentiment, paraphrase, similarity, and inference. We fine-tune RoBERTa-base (Liu et al., 2019) model for each task individually and report the results on the GLUE dev set.

Here the baseline non-flat optimizer and SWA are never among the most accurate. Both SAM and WASAM are the best in all but two (different) cases, only one of which is worse than the baseline.

### 5.3. Graph Representation Learning

We use a subset of the Open Graph Benchmark (OGB) datasets (Hu et al., 2020). The tasks are node property pre-
Table 2. NLP test results: Open-Domain Question Answering and Natural Language Understanding (GLUE) including paraphrase, sentiment analysis, and textual entailment.

| Task         | Model       | Baseline | SWA | SAM | WASAM |
|--------------|-------------|----------|-----|-----|-------|
| NQ           | FiD         | 49.35 ±0.44 | −0.20±0.13 | +0.33±0.19 | +0.48±0.22 |
| TriviaQA      | FiD         | 67.74 ±0.20 | +0.41±0.24 | +0.89±0.03 | +0.92±0.10 |
| COLA          | RoBERTa     | 60.41 ±0.22 | +0.09±0.04 | +1.57±0.20 | +1.41±0.14 |
| SST           | RoBERTa     | 94.95 ±0.11 | −0.30±0.07 | −0.29±0.46 | +0.19±0.14 |
| MRPC          | RoBERTa     | 89.14 ±0.57 | +0.08±0.16 | +0.73±0.43 | +0.81±0.38 |
| STSB          | RoBERTa     | 90.40 ±0.02 | +0.00±0.00 | +0.38±0.17 | +0.35±0.10 |
| QQP           | RoBERTa     | 91.30 ±0.07 | +0.01±0.06 | +0.08±0.07 | +0.06±0.08 |
| MNLI          | RoBERTa     | 87.41 ±0.40 | +0.00±0.01 | +0.39±0.02 | +0.37±0.01 |
| QNLI          | RoBERTa     | 92.90 ±0.06 | −0.08±0.11 | +0.09±0.01 | +0.11±0.06 |
| RTE           | RoBERTa     | 80.09 ±0.23 | −0.23±0.20 | +0.70±0.05 | −0.46±0.12 |

Table 3. GRL test results: Node Property Prediction (NPP), Graph Property Prediction (GPP), and Link Property Prediction (LPP).

| Task         | Model       | Baseline | SWA | SAM | WASAM |
|--------------|-------------|----------|-----|-----|-------|
| NPP: Products | SAGE        | 77.39 ±0.18 | −0.17±0.22 | −0.02±0.13 | −0.14±0.15 |
| NPP: Products | DGCN        | 85.42 ±0.17 | +0.11±0.08 | −0.14±0.05 | −0.08±0.07 |
| NPP: Code2   | GCN         | 78.92 ±0.08 | +0.39±0.10 | +0.15±0.06 | +0.57±0.03 |
| NPP: Code2   | DGCN        | 73.59 ±0.13 | +0.48±0.14 | +0.08±0.05 | +0.53±0.05 |
| GPP: Code2   | GCN         | 16.04 ±0.00 | +0.70±0.11 | +0.36±0.06 | +0.93±0.15 |
| GPP: Molpcga | DGCN        | 15.73 ±0.11 | +0.83±0.11 | +0.57±0.09 | +1.10±0.09 |
| LPP: Biolg    | CP          | 28.10 ±0.11 | +0.40±0.14 | −0.33±0.14 | +0.33±0.16 |
| LPP: Biolg    | CompEx      | 25.65 ±0.13 | +1.90±0.20 | −0.13±0.14 | +1.35±0.12 |
| LPP: Citation | GCN         | 84.09 ±0.00 | +0.07±0.01 | +0.01±0.03 | +0.05±0.02 |
| LPP: Citation | SAGE        | 84.94 ±0.01 | +0.14±0.01 | −0.02±0.01 | +0.12±0.02 |

2. There are 15 cases where only one of SWA or SAM improves over the non-flat optimizer. In 11 of these cases, WASAM still improves over the baseline.

3. The non-flat baseline optimizer achieves the best performance only in 4 out of 12 self-supervised learning and 2 out of 12 graph experiments (6 out of 42 in total).

6. Limitations and Future Work

First, we are aware that some of the shared, fixed hyperparameter values we used in experiments may harm the effect of flat optimizers. For example, Chen et al. (2021a) note that SAM’s performance gains increase with the number of model parameters. In theory, the ideal experimental design includes tuning all hyperparameters independently for the non-flat optimizer, SWA, SAM, and WASAM. However, this design forces the number of required runs to grow exponentially in unique hyperparameters and quickly renders this benchmark infeasible. We consider the study of certain hyperparameter interactions to be important future work.

Second, there is a quickly-growing number of averaging and minmax methods that we have not investigated. For example, in the averaging category, concurrent to this work, we notice novel ways to determine the averaging period and frequency (Cha et al., 2021; Guo et al., 2022). On the minimax side, we observe new methods that primarily aim at two distinct goals: (a) to reduce the computational cost of SAM (Brock et al., 2021; Du et al., 2021; Liu et al., 2022), or (b) to further improve the perturbation approximation ε (Kwon et al., 2021; Zhuang et al., 2022; Zhou & Chen, 2021). We hypothesize that improvements in each method will still produce an improved method when combined.

Third, in general, we believe fruitful directions of research include designing: (a) optimizers that explicitly find basins where training loss flatness more directly corresponds to higher hold-out accuracy, (b) post-processing methods for existing optimization runs to move into flatter regions of these basins, (c) loss functions whose contours more tightly align with accuracy contours. The results point to which tasks would most benefit from improving these things: graph learning tasks would clearly benefit from improvements in (a) (as SAM is never among the best performing method), and language tasks would benefit if (b) is improved (as SWA is never among the best performing method).

Fourth, despite our best efforts to evaluate the optimizer on a broad range of benchmark tasks, there are still plenty of unexplored domains: generative modeling, uncertainty estimation, or reinforcement learning, to name a few.
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7. Conclusion

In this work, we benchmarked two representatives of flat-minima optimization methods on a diverse set of tasks (in data, learning settings, and model architectures). When they improved over the non-flat optimizers, we investigated what aspects of the training/test surfaces they were exploiting to achieve this. When they did not, we found common assumptions were broken (e.g., train and test loss minimizers being largely uncorrelated).

This investigation showed us that (a) each method found flat regions in different, orthogonal ways, and (b) there were still flat regions around SAM that could be exploited to further drive down test error. To reach these we proposed a simple idea: combine both flat minimization approaches. Doing so further improved generalization, an approach that performed at least as well as the worst flat minimizer in 39 out of 42 cases. This investigation points to directions that could further improve flat minimizers and approaches that would benefit practitioners right now, given the problem at hand.

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Appendix

A. Visualization details

For each model, we re-compute the batch norm statistics by one forward-pass over the training set before evaluating it.

**Linear interpolations**  To linearly interpolate between two sets of parameters $\theta$ and $\theta'$, we parameterize the line connecting these two points by choosing a scalar parameter $\alpha$, and defining the weighted average $\theta(\alpha) = (1 - \alpha) \theta + \alpha \theta'$.

**2D Surface visualizations**  We choose the optimizer solution $\theta$ as center point of the plot, and two direction vectors, $\delta$ and $\eta$. Then, we plot the losses summed over the full training/test set as

$$f(\alpha, \beta) = \mathcal{L}(\theta + \alpha \delta + \beta \eta).$$

To yield $\delta$, $\eta$, we first sample $\delta, \eta \sim \mathcal{N}(0, I)$, orthogonalize $\eta$ w.r.t. to $\delta$ using the Gram-Schmidt process (Deisenroth et al., 2020), and then filter-wise normalize them (Li et al., 2018). For both training settings (WRN on CIFAR100, and GIN on Code2), we use $\alpha, \beta \in [-1, 1]$. For WRN on CIFAR100, we discretize the 2D-grid 20 with equally-spaced steps in each dimension; for GIN on Code2 with 15 steps. For better readability, we cropped the WRN on CIFAR100 plots shown in Figure 3 after computing the losses.

B. Experimental details

B.1. Computer Vision

We mostly adapt the hyper-parameter values from Foret et al. (2021) for WRN-28-10 and PyramidNet-272, from Dosovitskiy et al. (2021) for ViT, and from (Tolstikhin et al., 2021) for MLP-Mixer models. We average all results across three random seeds.

B.1.1. SUPERVISED CLASSIFICATION

We train WideResNets (Zagoruyko & Komodakis, 2016) with 28 layers and width 10 (WRN28-10) and PyramidNet (Han et al., 2017) with 110 layers and widening factor $\alpha = 272$ (PyramidNet-272) from scratch. The Vision Transformer (ViT) base model with input patch size 16 (ViT-B/16) and MLP-Mixer base model with input patch size 16 (MLP-Mixer-B/16) start from pre-trained checkpoints available at https://console.cloud.google.com/storage/vit/models/. The reason for using pre-trained checkpoints for the ViT and MLP-Mixer models is that, due to their lack of some inductive biases inherent to CNNs, such as translation equivariance and locality, they do not generalize well when trained on insufficient amounts of data (Dosovitskiy et al., 2021). Table 4 shows the hyper-parameters for each architecture.

Table 5 shows the hyper-parameters for each SSL method. We use implementations from the lightly package, available at https://github.com/lightly-ai/lightly (Susmelj et al., 2020).

B.2. Natural Language Processing

For the task of Open Domain Question Answering, we adapt the hyper-parameter values and the 100 retrieved passages for each question from Izacard & Grave, 2021. We report the Exact Match score of FiD-base model on Natural Questions (NQ) and TriviaQA test sets. For GLUE benchmark, we report Matthew’s Corr for CoLA, Pearson correlation coefficient for STSB, and accuracy for the the rest of the datasets. Results are all evaluated on the dev set of GLUE benchmark. We use the RoBERTa-base as our backbone language model, implemented with Huggingface Transformers (Wolf et al., 2020). Most of the task-specific hyper-parameter values are adapted from Aghajanyan et al., 2020.
### Table 4. Hyper-parameters for Supervised Classification (SC): CIFAR-{10, 100} (Table 1)

| Hyper-Parameter      | WRN28-10 | PyramidNet-272 | ViT-B/16 | MLP-Mixer-B/16 |
|----------------------|----------|----------------|----------|----------------|
| Base Optimizer       | SGD      | SGD            | SGD      | SGD            |
| Batch size           | 256      | 256            | 100      | 170            |
| Data augmentation    | Inception-style + Cutout (Devries & Taylor, 2017) | | | |
| Dropout rate         | 0.0      |                |          |                |
| Epochs               | 200      | 200            | –        | –              |
| Gradient clipping norm| –        | –              | 1.0      | 1.0            |
| Learning rate schedule| cosine  |                |          |                |
| Peak learning rate   | 0.1      | 0.05           | 0.03     | 0.03           |
| Steps                | –        | –              | 12500    | 12500          |
| SGD Momentum         | –        |                | 0.9      |                |
| Warmup steps         | –        |                | 500      | 500            |
| Weight decay         | 5e − 4   | 5e − 4         | 0.0      | 0.0            |

#### CIFAR-10

| Hyper-Parameter      | SAM ρ | Averaging start E (SWA) | Averaging start E (WASAM) |
|----------------------|-------|-------------------------|---------------------------|
|                      | 0.05  | 60%                     | 90%                       |
|                      | 0.05  | 60%                     | 75%                       |
|                      | 0.1   | 75%                     | 90%                       |
|                      | 0.1   | 60%                     | 75%                       |
|                      | 0.2   | 75%                     | 90%                       |
|                      | 0.05  | 90%                     | 90%                       |
|                      | 0.01  | 75%                     | 90%                       |
|                      | 0.01  | 90%                     | 90%                       |

#### CIFAR-100

| Hyper-Parameter      | SAM ρ | Averaging start E (SWA) | Averaging start E (WASAM) |
|----------------------|-------|-------------------------|---------------------------|
|                      | 0.1   | 60%                     | 90%                       |
|                      | 0.1   | 60%                     | 75%                       |
|                      | 0.2   | 75%                     | 90%                       |
|                      | 0.05  | 90%                     | 90%                       |
|                      | 0.01  | 75%                     | 90%                       |
|                      | 0.01  | 90%                     | 90%                       |

### Table 5. Hyper-parameters for Self-Supervised Learning (SSL): CIFAR-10, ImageNette, results in (Table 1)

| Hyper-Parameter      | MoCo   | SimCLR | SimSiam | BarlowTwins | BYOL   | SwaV   |
|----------------------|--------|--------|---------|-------------|--------|--------|
| Backbone Network     | SimCLR |        |         |             |        |        |
| Base Optimizer       | SGD    | Adam   |         |             |        |        |
| Data augmentation    |        |        |         |             |        |        |
| Dropout rate         |        |        | 0.9     |             |        |        |
| Epochs               |        |        | 800     |             |        |        |
| Embedding dimensions |        |        | 512     |             |        |        |
| KNN memory bank size |        |        | 4096    |             |        |        |
| Learning rate schedule|        |        | cosine  |             |        |        |
| Peak learning rate   |        |        | 6e − 2  |             | 1e − 3 |        |
| SGD Momentum         | 0.9    | –      | –       |             | –      | –      |
| Weight decay         |        |        | 5e − 4  |             | 1e − 6 |        |

#### CIFAR-10

| Hyper-Parameter      | Batch size | Crop size | Gaussian blur | Averaging start E (SWA) | Averaging start E (WASAM) |
|----------------------|------------|-----------|---------------|-------------------------|---------------------------|
|                      | 512        | 32        | 0%            | 75%                     | 90%                       |
|                      | 0.01       | 0.01      | 0.01          | 90%                     | 90%                       |
|                      | 0.05       | 0.01      | 0.03          | 90%                     | 75%                       |
|                      | 0.05       | 0.01      | 0.03          | 90%                     | 75%                       |
|                      | 0.05       | 0.05      | 0.01          | 75%                     | 90%                       |

#### ImageNette

| Hyper-Parameter      | Batch size | Crop size | Gaussian blur | SAM ρ | Averaging start E (SWA) | Averaging start E (WASAM) |
|----------------------|------------|-----------|---------------|-------|-------------------------|---------------------------|
|                      |            | 256       | 50%           | 0.01  | 50%                     | 90%                       |
|                      |            |           | 50%           | 0.01  | 50%                     | 90%                       |
|                      |            |           | 50%           | 0.02  | 50%                     | 90%                       |
|                      |            |           | 50%           | 0.05  | 50%                     | 90%                       |
|                      |            |           | 50%           | 0.05  | 50%                     | 90%                       |
B.3. Graph Representation Learning

We mostly adapt the hyper-parameter values from Hu et al. (2020) for GCN (Kipf & Welling, 2017), SAGE (Hamilton et al., 2017), and GIN (Xu et al., 2019), from Chen et al. (2021b) for (Lacroix et al., 2018) and ComplEx (Trouillon et al., 2016), and from Li et al. (2020) for DGCN. Due to high standard errors, we averaged the results of a few tasks more than three times, as mentioned in the following tables.

| Hyper-Parameter | SAGE | DGCN |
|-----------------|------|------|
| **NPP: OGB-Proteins** |      |      |
| Aggregation method | Mean | Softmax |
| Base optimizer | Adam | Adam |
| Convolution layer | SAGE | DyResGEN |
| Dropout rate | 0.0 | 0.1 |
| Hidden dimensions | 256 | 64 |
| Learning rate | 0.01 | 0.001 |
| Normalization layer | – | Layer norm |
| Number of epochs | 2000 | 1000 |
| Number of layers | 3 | 112 |
| Number of random seeds | 5 | 3 |
| Training cluster number | 1 | 15 |
| Weight decay | 0.0 | 0.0 |
| SAM $\rho$ | 0.01 | 0.02 |
| Averaging start $E$ (SWA) | 90% | 90% |
| Averaging start $E$ (WASAM) | 90% | 90% |

| **NPP: OGB-Products** |      |      |
| Aggregation method | Mean | Softmax |
| Base optimizer | Adam | Adam |
| Batch size | 20000 | – |
| Convolution layer | SAGE | Gen |
| Dropout rate | 0.5 | 0.5 |
| Evaluation cluster number | – | 8 |
| Learning rate | 0.01 | 0.001 |
| Hidden dimensions | 256 | 128 |
| Normalization layer | – | Batch norm |
| Number of epochs | 30 | 50 |
| Number of layers | 3 | 14 |
| Number of random seeds | 5 | 3 |
| Training cluster number | – | 10 |
| Weight decay | 0.0 | 0.0 |
| SAM $\rho$ | 0.01 | 0.02 |
| Averaging start $E$ (SWA) | 90% | 60% |
| Averaging start $E$ (WASAM) | 75% | 90% |
Table 7. Hyper-parameters for GPP: OGB-Code2, results in Table 3.

| Hyper-Parameter | GCN  | GIN  |
|-----------------|------|------|
| **GPP: OGB-Code2** |      |      |
| Aggregation method | Mean | Mean |
| Base optimizer | Adam | Adam |
| Batch size | 128  | 128  |
| Convolution layer | GCN  | GIN  |
| Dropout rate | 0.0  | 0.0  |
| Learning rate | 0.001 | 0.001 |
| Hidden dimensions | 300  | 300  |
| Normalization layer | Batch norm | Batch norm |
| Number of random seeds | 3 | 3 |
| Number of epochs | 15 | 30 |
| Number of layers | 5 | 5 |
| Virtual node embeddings | True | True |
| Vocabulary size | 5000 | 5000 |
| Weight decay | 0.0 | 0.0 |
| SAM $\rho$ | 0.2 | 0.15 |
| Averaging start $E$ (SWA) | 50% | 50% |
| Averaging start $E$ (WASAM) | 50% | 50% |

Table 8. Hyper-parameters for GPP: OGB-Molpcba, results in Table 3.

| Hyper-Parameter | GIN  | DGCN |
|-----------------|------|------|
| **GPP: OGB-Molpcba** |      |      |
| Aggregation method | Mean | Mean |
| Batch size | 512 | 512 |
| Base optimizer | Adam | Adam |
| Convolution layer | GIN | GEN |
| Dropout rate | 0.0 | 0.2 |
| Learning rate | 0.001 | 0.001 |
| Normalization layer | Batch norm | Batch norm |
| Number of epochs | 100 | 50 |
| Number of layers | 5 | 14 |
| Number of random seeds | 3 | 3 |
| Hidden dimensions | 300 | 256 |
| Virtual node embeddings | False | True |
| Weight decay | 0.0 | 0.0 |
| SAM $\rho$ | 0.01 | 0.15 |
| Averaging start $E$ (SWA) | 90% | 75% |
| Averaging start $E$ (WASAM) | 90% | 50% |
Table 9. Hyper-parameters for LPP: OGB-Biokg, results in Table 3.

| Hyper-Parameter | CP          | ComplEx     |
|-----------------|-------------|-------------|
| **GPP: OGB-Biokg** |             |             |
| Base optimizer  | Adam        | Adam        |
| Batch size      | 500         | 500         |
| Learning rate   | 0.1         | 0.1         |
| Number of random seeds | 3      | 3           |
| Number of epochs | 30         | 50          |
| Rank            | 1000        | 1000        |
| Regularizer     | N3          | N3          |
| Weight decay    | 0.0         | 0.0         |
| SAM ρ           | 0.1         | 0.05        |
| Averaging start E (SWA) | 50%     | 50%         |
| Averaging start E (WASAM) | 90%    | 50%         |

Table 10. Hyper-parameters for LPP: OGB-Citation2, results in Table 3.

| Hyper-Parameter | GCN          | SAGE        |
|-----------------|--------------|-------------|
| **GPP: OGB-Citation2** |             |             |
| Aggregation method | Mean        | Mean        |
| Base optimizer   | Adam         | Adam        |
| Batch size       | 256          | 512         |
| Convolution layer | GCN         | SAGE        |
| Dropout rate     | 0.0          | 0.2         |
| Hidden dimensions | 256         | 256         |
| Number of epochs | 300          | 300         |
| Number of layers | 3            | 3           |
| Number of random seeds | 3      | 3           |
| Normalization layer | –           | –           |
| Learning rate    | 0.001        | 0.0005      |
| Virtual node embeddings | False | False      |
| Weight decay     | 0.0          | 0.0         |
| SAM ρ            | 0.02         | 0.01        |
| Averaging start E (SWA) | 75%      | 90%         |
| Averaging start E (WASAM) | 60%    | 90%         |