Introduction to Machine Learning (for AI)

Regularization

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Today's Lecture

- Today we cover regularization, a way to control model complexity in a way that improves learning.
- Regularization is the main tool we use to combat overfitting and improve generalization.
- There are many ways to do regularization, in this lecture we cover the most common ones: weight penalization in the loss function.
- We also cover a little of multi-task learning

Outline

Regularization

It is a way to "guide" or introduce additional information to the learning process in order to reduce overfitting and improve generalization.

- Learning a function mapping from a set of data points is not trivial due to the number of degrees of freedom (N, D, P).
- Given N samples of D-dimensional features, if $N < D$ then the problem is called "ill-posed" or "ill-conditioned", as not all possible feature values are defined.

Regularization

- Usually you need $N >> D$ in order to learn a concept properly, but it can still be done if additional information is provided.
- Also if a model has P learnable parameters, then if $P > N$ not all model parameters have unique values. This is called an underspecified problem.
- Even if $P < N$ or $N < D$ a concept can still be learned, if additional information to the learning process is provided in order to obtain unique solutions.

Regularization

- But while unique solutions are desirable in theory, in practice they are not necessarily "better". Deep Neural Networks have multiple solutions and theory has proven that these are quite similar to each other.
- The relationship between all these variables is not completely understood, specially the relation between P and N, D, as the amount of information in each training sample might offset having a small sample size (for example, large images).

Big Question

The biggest question related to the previous points is:

How do we add additional information to the learning process?

This sounds simple in concept but implementing is very difficult.

Regularization

Concept

Regularization is to constraint the model to limit its learning capacity and/or complexity, so it is under the control of the ML user.

Usually this is achieved by putting constraints on the weight values, limiting the expressiveness and effective number of parameters (similar to P).

Advanced methods used in Neural Networks put constraints on activations (Batch Normalization) or introduce noise into the learning process (Dropout). But we do not cover it in this course.

Regularization - General Patterns

Some general concepts or patterns for regularization methods:

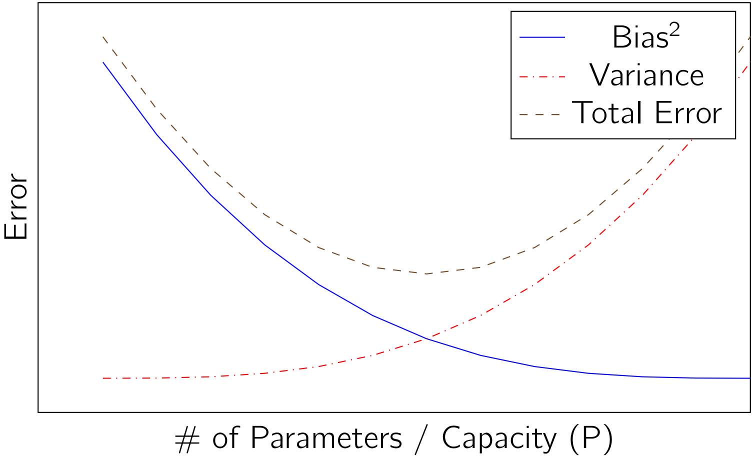
Weight Constraints Put limitations into weight values, reducing the effective number of parameters.

Output Constraints Put limitations into intermediate or final output values, also reducing the effective number of parameters.

Introducing Noise Add noise to features or weights to constraint undesirable interactions like correlations between features.

In all cases, the model equations are constrained somehow.

Relation with Bias-Variance Trade-off



Relation with Bias-Variance Trade-off

- When regularizing a model, the complexity/capacity P changes.
- Regularization methods typically have a strength parameter (let's call it R), that implicitly controls model complexity/capacity.
- The new model complexity/capacity is called the effective P and depends on the regularization strength.

Relation with Bias-Variance Trade-off

Large R	Big regularizing effect, model is very constrained, and effective P decreases significantly.
Middle R	Balanced regularization effect, model is constrained but not too much, potential improvement in generalization. Effective P is smaller than P.
Small R	Almost no regularization effect, model is not or little constrained, and effective P is almost the same as P.

Outline

Early Stopping

- Usually iterative methods are used to train machine learning models. Then the number of iterations (or epochs) becomes a tunable hyper-parameter.
- As we saw in bias-variance trade-off, there is usually a point where the model starts to overfit.
- Early stopping is just the process of stopping training right before the validation loss starts to increase. Most ML frameworks implement this mechanism.
- An important points is that to do this one needs a three-way split (train/val/test), as choosing the stopping point counts as hyper-parameter tuning, and only evaluation on a test will be unbiased.

L^p Regularization (Tikhonov's)

It is the most common regularization method. It consists of introducing a penalty that considers the norm of the model parameters (weights):

$$L^*(f(x), y) = L(f(x), y) + \lambda \sum_i |w_i|^p \tag{1}$$

The sum is over all trainable model parameters. The regularization coefficient λ is a hyperparameter that defines the strength of regularization. p is the norm dimensionality, typically set to 1 (called LASSO) or 2 (weight decay). This method heavily restricts the capacity of the model, achieving better generalization.

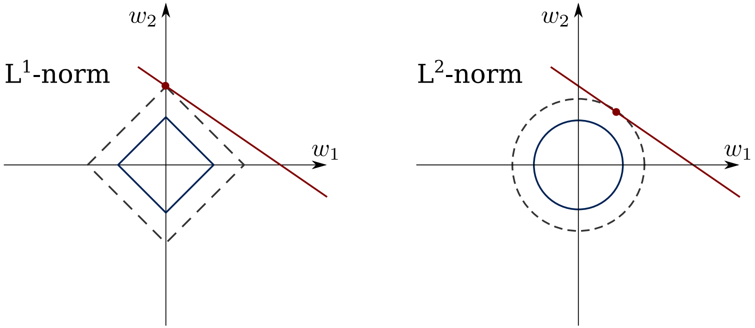
L^1 Regularization (LASSO)

- It has the tendency to make some of the model parameters to be set to zero (a sparse solution).
- A model parameter will be non-zero only if it positively contributes to reduce the original loss of the model, in a way to "counter-act" the penalty from the regularization term.
- If used with a linear model, inputs associated to non-zero weights can be interpreted as relevant features, which constitutes a feature selection method.

L^2 Regularization (Weight Decay)

- Tends to make the model's parameters decay to small values, unless they are supported by the data and reduce the loss of the model.
- Early stopping is related to Weight Decay, as weights usually grow with time (iterations). Doing Early Stopping controls how much the weights can grow, effectively decaying them.
- Both regularization methods have a Bayesian point of view, which corresponds to setting a prior distribution on the model parameters.
- L^2 regularization improves convexity of the loss function.

Geometric Interpretation of L^1 and L^2 Regularization



This shows that L1 regularization produces sparse weights, while L2 regularization decreases the values of the weights (decaying).

Figure from `https://en.wikipedia.org/wiki/Regularization_(mathematics)`

Elastic Net Regularization

L^1 regularization has some disadvantages, like oversparsification of weights, or selecting up to N weights if N is small (number of training samples.

An alternative is Elastic Net, which combines L^1 and L^2 regularization:

$$L^*(f(x), y) = L(f(x), y) + \lambda_1 \sum_i |w_i| + \lambda_2 \sum_i w_i^2 \quad (2)$$

Now there are two regularization strength coefficients λ_1 and λ_2, that need to be adjusted.

Regularization in Linear Regression

Regularization can be used in LR to control model complexity, by adding a term in the loss:

$$L = n^{-1}(\mathbf{y} - W\mathbf{X})^T(\mathbf{y} - \mathbf{X}W) + \lambda ||W||^p \tag{3}$$

Then the gradient is:

$$\frac{\partial L}{\partial W} = n^{-1}\mathbf{X}^T(\mathbf{X}W - \mathbf{y}) + \lambda p ||W||^{p-1} \tag{4}$$

Regularization in Linear Regression

For L2 regularization ($p = 2$) we have:

$$\frac{\partial L}{\partial W} = n^{-1}\mathbf{X}^T(\mathbf{X}W - \mathbf{y}) + \lambda 2||W|| \tag{5}$$

And for L1 regularization ($p = 1$):

$$\frac{\partial L}{\partial W} = n^{-1}\mathbf{X}^T(\mathbf{X}W - \mathbf{y}) + \lambda \tag{6}$$

Regularization in Linear Regression

For L2 regularization ($p = 2$), the closed form solution has a nice form:

$$W = (n^{-1}\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y} \tag{7}$$

Here the added term λI controls how invertible the whole term $\mathbf{X}^T\mathbf{X} + \lambda I$ is.

For example if there are correlated variables, using the regularization coefficient λ might help the term be invertible (it is not if there are correlated variables).

Regularization in Linear Regression

Another interpretation is that the value of λ controls between bias and variance of your solution, with $\lambda = 0$ this is equivalent to not using regularization, while high values of λ might produce very biased solutions that don't fit your data.

Remeber that the value of λ should always be tuned using cross validation in validation set. λ is your regularization strength coefficient (R).

Regularized Logistic Regression

Logistic Regression can also be regularized using L1 and L2 regularization. The loss now looks like:

Binary Cross-Entropy

$$L(y, \hat{y}) = -\sum_i y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i) + \lambda ||w||^p \tag{8}$$

Categorical Cross-Entropy

$$L(y, \hat{y}) = -\sum_i \sum_c y_i^c \log(\hat{y}_i^c) + \lambda ||w||^p \tag{9}$$

SVM Regularization

Regularization in support vector machines is controlled by the C coefficient in the soft margin formulation:

$$L = ||\mathbf{w}|| + C \sum_i \max(0, 1 - y_i(\mathbf{w}\mathbf{x}_i + b)) \tag{10}$$

In Scikit-learn, the regularization strength has a inverse relationship with the C coefficient (i.e. $R = C^{-1}$).

If using the hard margin formulation, it is also possible to add L1 or L2 regularization penalties to the standard SVM loss formulation.

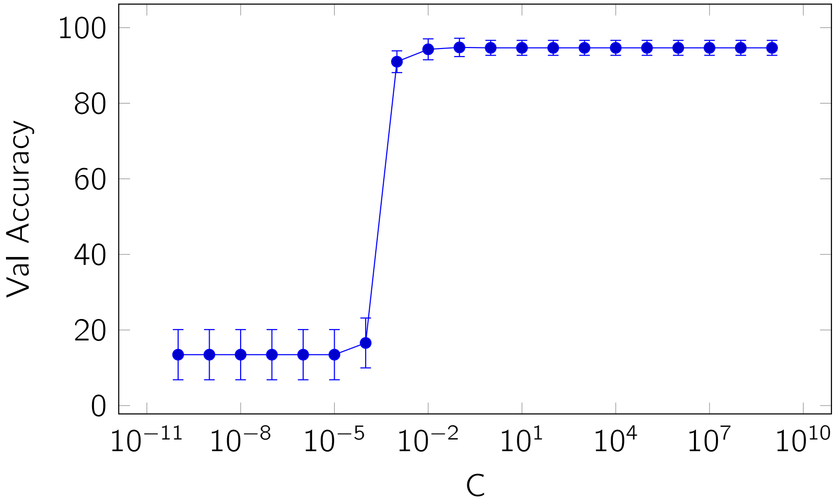
Tuning the regularization coefficient λ

- λ can be used to control the effective model capacity.
- If λ is too large, the model will underfit, and if λ is too small, then regularization is not efficient and the model could overfit.
- One way to tune this parameter is through grid search. Create a grid of values in **logarithmic** scale, like: $\lambda \in [10^{-l}, \cdots, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}, 10^{1}, 10^{2}, 10^{3}, \cdots, 10^{l}]$.
- Then train a model for each value of λ and evaluate on a validation set. Use the model with the best validation performance, and make a final evaluation on the test set.

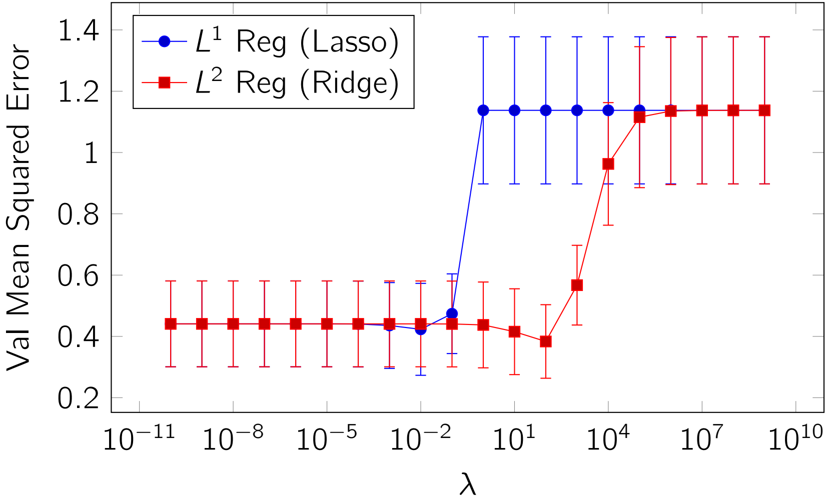
Tuning the regularization coefficient λ

- K-Fold Cross-validation is preferable in order to learn a more robust estimate of λ.
- The scale of λ depends on the scale of the loss function that is being regularized.
- Different losses have different ranges, for example, range of cross-entropy for classification depends on C (number of classes), while range of mean squared error for regression depends on the labels/model output ranges.
- This is a hyper-parameter tuning problem, you can use methods for the previous lecture.

Tuning λ example: 8×8 Digits SVM Classification



Tuning λ example: Boston Dataset Linear Regression



Output Regularization

- It is also possible to add regularization penalties to the output of your model, to constraint valid values.
- This is particularly useful for regression.
- Same L1/L2 regularization applies, but the penalty term uses model output instead of weights.

$$L^*(f(x), y) = L(f(x), y) + \lambda \sum_i |f(x)_i|^p \qquad (11)$$

- Here assuming $f(x)_i$ is the model output (a vector) over dimensions i.

Outline

What is Multi-Task Learning?

- Classical machine learning deals with learning a single task at a time. For example, doing classification or regression is a single task.
- But real world applications sometimes involve learning more than one task at the same time, for example, Object Detection requires both image classification and bounding box regression together.
- In general there are advantages to learning multiple tasks at the same time, as relations and common knowledge between tasks usually improves generalization performance.
- It has a regularizing effect :)

Multi-Task Learning - How?

The most simple way to perform multi-task learning is to use neural networks, as one can design an architecture that has multiple outputs (as desired), and typically a shared trunk of weights can indirectly encode common or shared knowledge.

Still we need a single loss function to optimize during learning. The most common approach is to linearly combine the loss for each task L_i. This requires labels for each task.

$$L(x, y, \theta) = \sum_i w_i L_i(f_i(x), y, \theta_i) \tag{12}$$

Where $f_i(x)$ is the output head of the i-th task, and this head has weights θ_i.

Multi-Task Learning - How?

The weights for each task w_i then have to be tuned in order to maximize performance.

The w_i's are hyper-parameters, so they can be tuned using methods from the previous lecture.

Note that the exact scale of the weights does not matter as multiplying the loss by a positive scalar does not change the optimum.

Multi-Task Learning - Hard Parameter Sharing

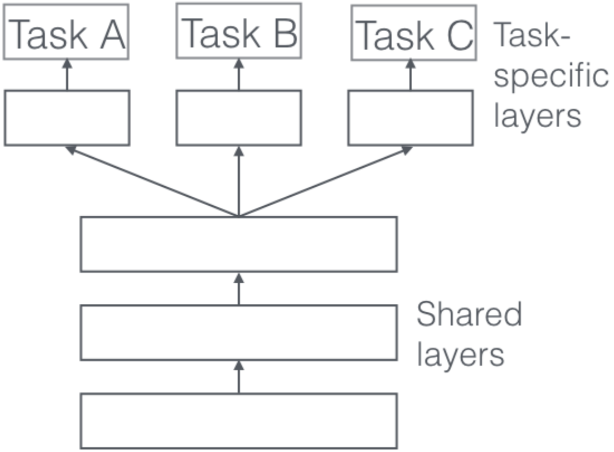
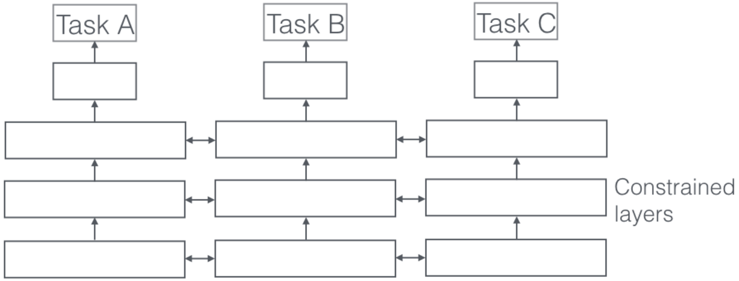


Figure taken from "An Overview of Multi-Task Learning in Deep Neural Networks" by Sebastian Ruder. http://ruder.io/multi-task/

Multi-Task Learning: Soft Parameter Sharing



Weights can be constrained by adding terms to the loss function, such as:

$$||W_A - W_B||^2 + ||W_A - W_C||^2$$

Figure taken from "An Overview of Multi-Task Learning in Deep Neural Networks" by Sebastian Ruder. http://ruder.io/multi-task/

Multi-Task Learning Performance: 1D-ALVINN Dataset

- This is dataset produced by a road simulator, where the principal task is to predict the steering angle from road conditions.
- The simulator is augmented to produce additional labels representing new tasks, namely: road is one or two lanes, left edge, center, and right edge road locations, location and intensity of road centerline, intensity of road surface and region bordering road.
- Neural networks of varying hidden units (HU) sizes are evaluated. The Root of Mean Squared Error for the steering angle is used for evaluation.

Multi-Task Learning Performance: 1D-ALVINN Dataset

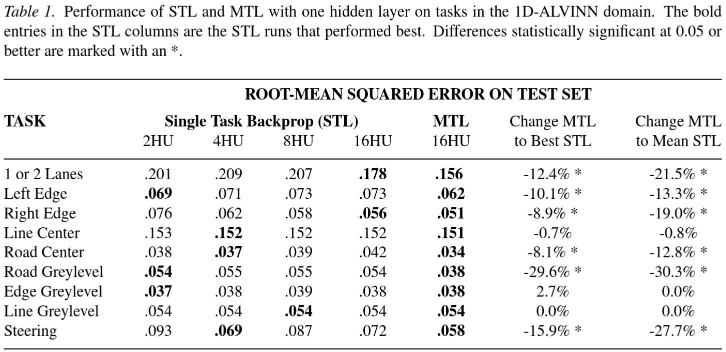


Table 1. Performance of STL and MTL with one hidden layer on tasks in the 1D-ALVINN domain. The bold entries in the STL columns are the STL runs that performed best. Differences statistically significant at 0.05 or better are marked with an *.

ROOT-MEAN SQUARED ERROR ON TEST SET

TASK	**Single Task Backprop (STL)**				**MTL**	Change MTL	Change MTL
	2HU	4HU	8HU	16HU	16HU	to Best STL	to Mean STL
1 or 2 Lanes	.201	.209	.207	**.178**	**.156**	-12.4% *	-21.5% *
Left Edge	**.069**	.071	.073	.073	**.062**	-10.1% *	-13.3% *
Right Edge	.076	.062	.058	**.056**	**.051**	-8.9% *	-19.0% *
Line Center	.153	**.152**	.152	.152	**.151**	-0.7%	-0.8%
Road Center	.038	**.037**	.039	.042	**.034**	-8.1% *	-12.8% *
Road Greylevel	**.054**	.055	.055	.054	**.038**	-29.6% *	-30.3% *
Edge Greylevel	**.037**	.038	.039	.038	**.038**	2.7%	0.0%
Line Greylevel	.054	.054	**.054**	.054	**.054**	0.0%	0.0%
Steering	.093	**.069**	.087	.072	**.058**	-15.9% *	-27.7% *

In pretty much all cases MTL performs better (lower RMSE) than using a single task (STL).

Figure taken from "Multi-Task Learning" by Rich Caruana. 1997.

Multi-Task Learning Performance - Drug Discovery

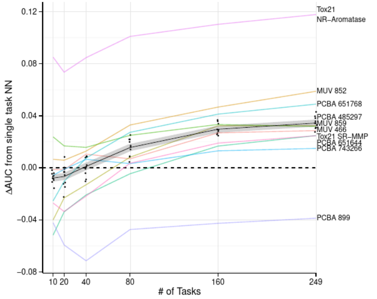


Figure 3. Held-in growth curves. The y-axis shows the change in AUC compared to a single-task neural network with the same architecture (PSTNN). Each colored curve is the multitask improvement for a given held-in dataset. Black dots represent means across the 10 held-in datasets for each experimental run, where additional tasks were randomly selected. The shaded curve is the mean across the 100 combinations of datasets and experimental runs.

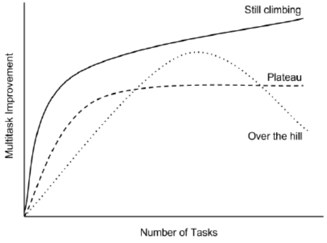


Figure 2. Potential multitask growth curves

Figures taken from "Massively Multitask Networks for Drug Discovery" by Ramsundar et al. 2015.

Multi-Task Learning Performance - Drug Discovery

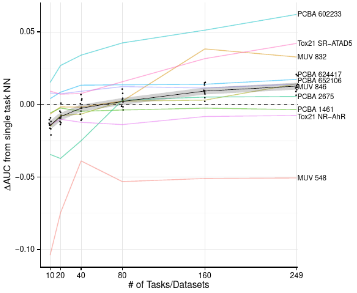


Figure 5. Held-out growth curves. The y-axis shows the change in AUC compared to a single-task neural network with the same architecture (PSTNN). Each colored curve is the result of initializing a single-task neural network from the weights of the networks from Section 4.2 and computing the mean across the 10 experimental runs. These datasets were *not* included in the training of the original networks. The shaded curve is the mean across the 100 combinations of datasets and experimental runs, and black dots represent means across the 10 held-out datasets for each experimental run, where additional tasks were randomly selected.

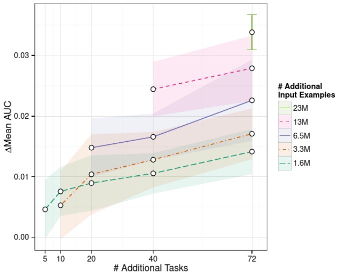


Figure 4. Multitask benefit from increasing tasks and data independently. As in Figure 2, we added randomly selected tasks (x-axis) to a fixed held-in set. A stratified random sampling scheme was applied to the additional tasks in order to achieve fixed total numbers of additional input examples (color, line type). White points indicate the mean over 10 experimental runs of Δ mean-AUC over the initial network trained on the 10 held-in datasets. Color-filled areas and error bars describe the smoothed 95% confidence intervals.

Figures taken from "Massively Multitask Networks for Drug Discovery" by Ramsundar et al. 2015.

Why does MTL Work?

Statistical Data Amplification / Data Augmentation

It is an effective increase in the size of the training set, as additional information flows from multiple tasks, which allows the learning process to "average-out" noise in the labels and in the inputs.

Attribute Selection

Some tasks are harder than others due to noise and high dimensionality, but another task can help the model to learn a shared feature that is harder to learn with a single task alone.

MTL effectively helps models focus into the most important features. It is a consequence of Data Amplification.

Why does MTL Work?

Eavesdropping

Given two tasks T_A and T_B that share a feature F, consider that F is harder to learn in one of the task. When performing Multi-Task Learning, one task can "eavesdrop" into the other as they share parameters, and we hope that the shared layers can learn F effectively.

There is extra information in one of the tasks that helps learn the feature representation for the other task. This means for example that if learning F through T_A is harder, when doing MTL, learning F through T_B might be easier.

Representation Bias

As MTL is performed, it introduces a bias to learn representations and features that also generalize for other tasks. This increases the chance that a good generalizable feature is learned.

Questions to Think About

1. Explain regularization in your own words (the concept).
2. Describe two general concepts for Regularization.
3. How to select the regularization strength coefficient $R/C/\lambda$?
4. What is the effect of decreasing/increasing the regularization strength R on under/overfitting?
5. How to apply regularization to a multi-class classification model (say multi-class LogReg)?
6. Why multi-task learning improves performance?

Take Home Messages

- Regularization is the whole field of constraining your model to increase generalization performance.
- Three ways to conceptually do regularization, constraint weights, constraint outputs, and introduce noise.
- Regularization methods have a strength parameter that controls the Bias-Variance trade-off.
- Multi-Task learning can also be used to improve performance at the expense of additional tasks.

Questions?