Regularization and Model Selection

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Underfitting and overfitting - intuition

Imagine that you have to study for a written exam consisting of exercises.

Doing only a few exercises while studying leads to poor perfomance both on homework and at the exam. This is called *underfitting*: the performance at the exam will be bad because of poor training.

Moreover, memorize all the solutions to homework leads to the maximum score on homework (trivially) but probably a bad score on the exam exercises. This is called *overfitting*: you have a bad performance on the exam because you did not capture the true essence of the homework, rather you have memorized their peculiarities.

Underfitting and overfitting - analytical example

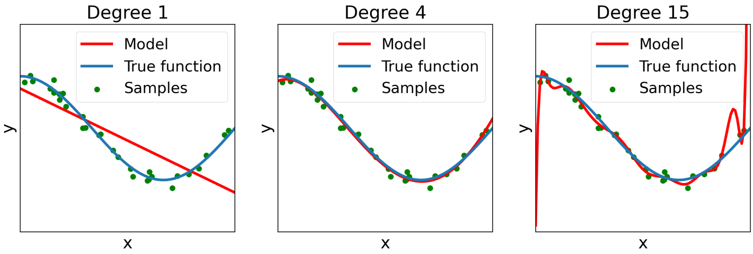


Figure: Underfitting (polynomial degree 1), good fitting (polynomial degree 4), overfitting (polynomial degree 15).

Overfitting can be countered through:

- regularization;
- validation.

Regularization

Overfitting is correlated with “complex” models: to avoid them, we penalize models with large weights. One way to do this is to consider the following cost function

$$E_r(\boldsymbol{w}) = E(\boldsymbol{w}) + R_\lambda(\boldsymbol{w})$$

where R_λ is the *regularization term*.
$\lambda > 0$ is a hyperparameter that must be chosen in the **model selection phase** (see later).

Most common regularization techniques:

- Tikhonov (or L^2 or *Ridge*): $R_\lambda(\boldsymbol{w}) = \lambda||\boldsymbol{w}||_2^2 = \lambda \sum_i w_i^2$. Tends to make *all* weights small.
- LASSO (or L^1): $R_\lambda(\boldsymbol{w}) = \lambda||\boldsymbol{w}||_1 = \lambda \sum_i |w_i|$. Tends to make *some* weights 0 (feature selection).

Linear Regression with Tikhonov regularization

- Cost function (without regularization):

$$E(\boldsymbol{w}) = \frac{1}{N}||\mathrm{X}\boldsymbol{w} - \boldsymbol{y}||^2$$

- Regularized cost function:

$$E_r(\boldsymbol{w}) = E(\boldsymbol{w}) + \lambda||\boldsymbol{w}||^2$$

- Gradient of the regularized cost function:

$$\nabla E_r(\boldsymbol{w}) = \nabla E(\boldsymbol{w}) + 2\lambda\boldsymbol{w} = 2\left(\frac{1}{N}\mathrm{X}^T(\mathrm{X}\boldsymbol{w} - \boldsymbol{y}) + \lambda\boldsymbol{w}\right)$$

- Normal equation:

$$\boldsymbol{w} = (\mathrm{X}^T\mathrm{X} + \lambda\mathrm{I})^{-1}\mathrm{X}^T\boldsymbol{y}$$

Note that in this case $\mathrm{X}^T\mathrm{X} + \lambda\mathrm{I}$ is *always* invertible (why?).

Bias-Variance trade-off

Bias: expected discrepancy between targets and predictions given by the model.

Variance: measure of the deviation from the expected value given by the model that any particular sampling of the data (from the same underlying data-generating distribution) is likely to cause.

Some intuitions on the effect of regularization:

- High $\lambda \rightsquigarrow$ simple model $\rightsquigarrow$ high bias (underfitting).
- Low $\lambda \rightsquigarrow$ complex model $\rightsquigarrow$ high variance (overfitting).
- Intermediate λ: optimal solution (good bias-variance trade-off).

Generalization

Central challenge in Machine Learning: **generalization**! Our algorithm must perform well on *new, previously unseen* inputs.

Recall that we have to find a balance between bias and variance. Even if we limit the complexity of our model using regularization, the training set does not provide a good estimate of the test (generalization) error.

In other words, generalization is compromised if we choose hyperparameters (including the regularization factor) only according to the training error.

Generalization - Training vs test error

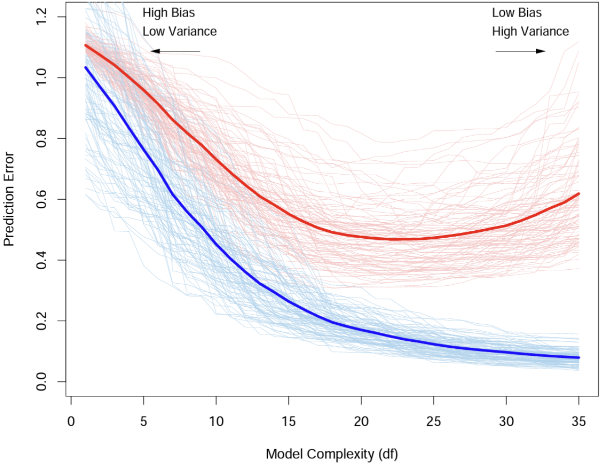


Figure: Training (blue) and test (red) errors as the model complexity varies.

Early stopping

- Store a copy of the model parameters every epoch the validation loss improves;
- if the validation loss does not improve for a fixed number of epochs (*patience*), terminate and return the best parameters.

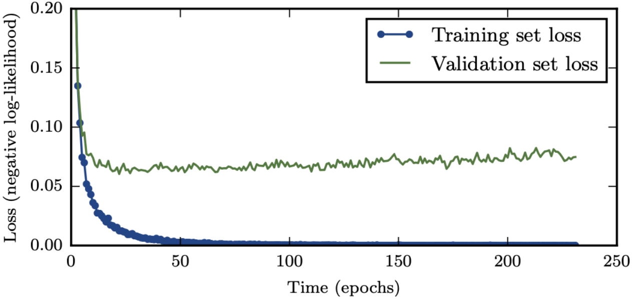


Figure: Learning curves for a classifier trained on the MNIST dataset.

Model selection and model assessment

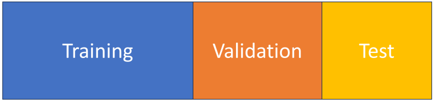
Do **not** use the test set to tune hyperparameters: introduce the **validation set**.

In general, we should distinguish between:

1. Model selection: estimate the performance of different models trained with different hyperparameters.
2. Model assessment: after choosing a final model we evaluate its performance on *new, previously unseen* (test) data.

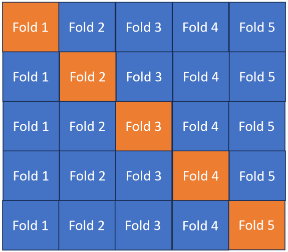
Once we have selected a model using the validation set, we can assess its generalization error on the test set. Splitting the dataset into training and validation sets is called *hold-out*.

Double Hold-out



- We split the entire dataset in three sets: training, validation and test (usually 60%-20%-20% or 70%-20%-10% of the total dataset).
- Training set is used to fit the model. Then, we evaluate its validation performance and adjust its hyperparameters to maximize it. We re-fit the model and keep adjusting the hyperparameters until we find a model with a good trade-off between training and validation performance.
- We assess the generalization capability of the best model by evaluating the performance on the test set.

Cross-Validation



Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Figure: 5-fold CV

- Split the data in k disjoint *folds*.
- Use $k-1$ folds as the training set and the remaining fold as the validation set. Repeat k times (see figure).
- The performance will be the mean $\pm$ standard deviation computed across the k runs.

Pro: Not sensitive to a particular partition of the data. Mean filter the error.
Cons: Computationally expensive (but parallellizable).

CV for selection and hold-out for assessment

1. Split dataset into two sets (hold-out): development D (model selection) and test T (model assessment).
2. Use the cross validation method on D to select the best model. *Optional*: retrain the best model using the entire dataset D.
3. Evaluate the generalization error on the test set T.

Grid search

How to choose the best set of hyperparameters?

Example: two hyperparameters (learning rate α and regularization parameter λ). Consider sets of three values for each parameter, e.g. $\alpha_{\text{vals}} = \{0.001, 0.01, 0.1\}, \lambda_{\text{vals}} = \{0.0001, 0.001, 0.01\}$. Evaluate the model with $(\alpha, \lambda) = (i, j)$ for $i \in \alpha_{\text{vals}}, j \in \lambda_{\text{vals}}$.

		λ	
	(0.001,0.0001)	(0.001, 0.001)	(0.001, 0.01)
α	(0.01, 0.0001)	(0.01, 0.001)	(0.01, 0.01)
	(0.1, 0.0001)	(0.1, 0.001)	(0.1, 0.01)

Choose the pair of value corresponding to the *best performance on the validation set*.

Refinement: Suppose that the best is $(0.1, 0.001)$. Then we can "zoom" near the best set doing another grid search with e.g. $\alpha_{\text{vals}} = \{0.075, 0.1, 0.125\}, \lambda_{\text{vals}} = \{0.00075, 0.001, 0.00125\}$.