Deep Learning Book

Chapter 7
Regularization for Deep Learning

Botian Shi
botianshi@bit.edu.cn

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Generalization and Strategy

- How to make an algorithm that will perform well not just on the training data, but also on new inputs?
- Many strategies designed to reduce the test error, possibly at the expense of increased training error.
- These strategies are known collectively as **regularization**.
- Many regularization algorithm have been developed.
- Developing more effective regularization strategies is one of the major research efforts in the field.
- In this chapter, we describe regularization in more detail, focusing on regularization strategies for deep models or models that may be used as building blocks to form deep models.

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Generalization and Strategy

- There are many regularization strategies.
  1. Put extra constrains on a machine learning model. (Adding restrictions on the parameter values.)
  2. Add extra terms in the objective function that can be thought of as corresponding to a soft constraint on the parameter values.
- If chosen carefully, these extra constraints and penalties can lead to improved performance on the test set.
- Sometimes these constraints and penalties are designed to
  1. **encode** specific kinds of **prior knowledge**.
  2. Express a generic preference for a simpler model class in order to promote generalization.
  3. make an under-determined problem determined. (Provide more information)
- Other forms of regularization, known as ensemble methods, combine multiple hypotheses that explain the training data.

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Generalization and Strategy

- Principle: Treading increased bias for reduced variance.
- An effective regularizer is one that makes a profitable trade, **reducing variance** significantly while not overly **increasing the bias**.
- In practice, **an overly complex model family does not necessarily include the target function or the true data generating process, or even a close approximation**.
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Generalization and Strategy

- However, most applications of deep learning algorithms are to domains where the true data generating process is almost certainly outside the model family.
- Deep learning algorithms are typically applied to **extremely complicated domains** such as images, audio sequences and text, for which the true generation process essentially involves **simulating the entire universe**.
- To some extent, we are always trying to fit a square peg(the data generating process) into a round hole (our model family) 『持方枘 (ruì) 而欲内圆凿』.
- What this means is that controlling the complexity of the model is not a simple matter of finding the model of the right size, with the **right number of parameters**.
- Insteamd, we might find that the best fitting model is a large model that has been regularized appropriately.
- We now review several strategies for how to create such a large, deep, regularized model.

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Parameter Norm Penalties

- Regularization has been used for decades prior to the advent of deep learning.
- Linear models allow simple straightforward and effective regularization strategies.
- Most approaches are based on limiting the capacity of models by adding a **parameter norm penalty** $\Omega(\theta)$ to the objective function J:

$$\tilde{J}(\boldsymbol{\theta}; X, y) = J(\boldsymbol{\theta}; X, y) + \alpha\Omega(\boldsymbol{\theta})$$

  where $\alpha \in [0, +\infty)$ weights the relative contribution of the norm penalty term.
- Setting α to 0 results in no regularization. Larger values of α correspond to more regularization.
- Optimize both J and norm
- Different Ω has different result.

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- We penalize **only the weights** of the affine transformation at each layer and leaves the biases unregularized.
- We do not induce too much variance by leaving the biases unregularized.
- Regularizing the bias parameters can introduce a significant amount of under-fitting.
- We therefore use the vector $\boldsymbol{w}$ to indicate all of the weights that should be affected by a norm penalty, while the vector $\boldsymbol{\theta}$ denotes all of the parameters, including both $\boldsymbol{w}$ and the unregularized parameters.
- Sometime we use a separate penalty with a different α coefficient for each layer.
- But it can be expensive to search for the correct value of multiple hyper-parameters, it is still reasonable to use the same weight decay at all layers just to reduce the size of search space.

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L^2 Parameter Regularization

- The L^2 norm penalty commonly known as *weight decay*.

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2}\|w\|_2^2$$

- This regularization strategy drives the weights closer to the origin. (as well as *ridge regression* or *Tikhonov regularization*)
- We can gain some insight into the behavior of weight decay regularization. (assume no bias for simplification)

$$\tilde{J}(w; X, y) = \frac{\alpha}{2} w^T w + J(w; X, y)$$

$$\nabla_w \tilde{J}(w; X, y) = \alpha w + \nabla_w J(w; X, y)$$

- The update

$$w \leftarrow w - \epsilon(\alpha w + \nabla_w J(w; X, y))$$

$$w \leftarrow (1 - \epsilon\alpha) w - \epsilon \nabla_w J(w; X, y)$$

- Shrink the weight vector by a constant factor on each step.
- What happens over the entire course of training?

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Recall: Quadratic Approximation

- In mathematics, approximation theory is concerned with how functions can best be approximated with simpler functions.
- **local linear approximation** and **taylor expansion**
  1. For example, when the independent variable of function $y = x^3$ changes, which is Δx, the variation of y is

$$\Delta y = (x + \Delta x)^3 - x^3 = 3x^2 \Delta x + 3x(\Delta x)^2 + (\Delta x)^3$$

  2. When $\Delta x \to 0$, omit last two terms: $\Delta y = 3x^2 \Delta x$
  3. In general:

$$\Delta y = f(x_0 + \Delta x) - f(x_0) \approx f'(x_0) \times \Delta x$$

$$\Delta y = f(x) - f(x_0),\ \Delta x = x - x_0$$

$$f(x) - f(x_0) = f'(x_0) \times (x - x_0)$$

$$f(x) = f(x_0) + f'(x_0)(x - x_0)$$

  4. In order to improve the precision, we can use second-order approximation, which is the second-order Taylor series expansion.

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2$$

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$$f(x) = f(x_0) + f'(x_0)(x - x_0)$$

  4. In order to improve the precision, we can use second-order approximation, which is the second-order Taylor series expansion.

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Recall: Quadratic Approximation

- In mathematics, approximation theory is concerned with how functions can best be approximated with simpler functions.
- **local linear approximation** and **taylor expansion**
  1. For example, when the independent variable of function $y = x^3$ changes, which is Δx, the variation of y is

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L^2 Parameter Regularization

- Let $w^* = \arg\min_w J(w)$ (unregularized training cost)
- Making a quadratic approximation to the objective function in the neighborhood of the value of the weights. (In DLBook, they used $\hat{J}(\boldsymbol{\theta})$, but here we use $\hat{J}(w)$ to explain easier)

$$\hat{J}(w) = J(w^*) + \frac{1}{2}(w - w^*)^T \mathrm{H}(w - w^*)$$

- Where H is the Hessian matrix of J with respect to w evaluated at w^*.
- There is no first-order term in this quadratic approximation, because w^* is defined to be a minimum, where the gradient vanishes.
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- To study the effect of weight decay, we modify $\nabla_w \hat{J}(w) = \mathsf{H}(w - w^*)$ by adding the weight decay gradient.
- We can solve for the minimum of the regularized version of $\hat{J}$.
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$$\alpha \tilde{w} + \mathsf{H}(\tilde{w} - w^*) = 0$$

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$$\tilde{w} = \frac{\mathsf{H}w^*}{(\mathsf{H} + \alpha \mathsf{I})}$$

- As α approaches 0, the regularized solution $\tilde{w}$ approaches w^*.
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- Because H is real and symmetric, we can decompose it into a diagonal matrix $\mathbf{\Lambda}$ and an orthonormal basis of eigenvectors, Q, such that $\mathrm{H} = Q\mathbf{\Lambda}Q^T$.
- Applying the decomposition $\tilde{w} = (\mathrm{H} + \alpha \mathrm{I})^{-1}\mathrm{H}w^*$

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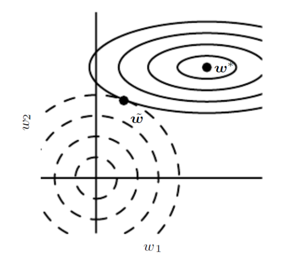
This effect is illustrated in figure:

Fig. 1: An illustration of the effect of L^2 (or weight decay) regularization on the value of the optimal w



- The solid ellipses represent contours of equal value of the **unregularized objective**.
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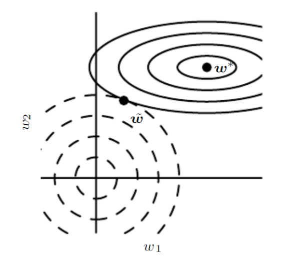

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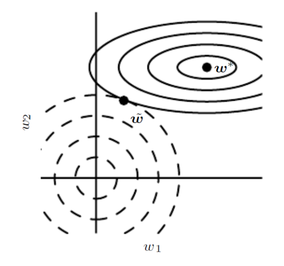

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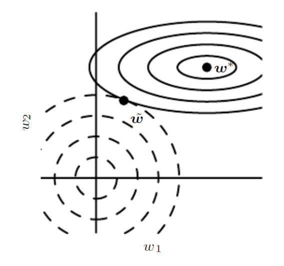

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L^2 Parameter Regularization

- How do these effects relate to machine learning in particular?
- We can find out by studying linear regression, the cost function is the sum of squared errors:

$$(Xw - y)^T(Xw - y)$$

- Add L^2 regularization, the objective function changes to:

$$(Xw - y)^T(Xw - y) + \frac{1}{2}\alpha w^T w$$

- This changes the normal equations for the solution from:

$$w = (X^TX)^{-1}X^Ty \text{ to } w = (X^TX + \alpha I)^{-1}X^Ty$$

- The new matrix has the addition of α to the diagonal.
- Diagonal correspond to the variance of each input feature.
- We can see that L^2 regularization causes the learning algorithm to "perceive" the input X as having higher variance, which makes it shrink the weights on features whose covariance with the output target is low compared to this added variance.

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L^1 Regularization

- L^1 regularization on the model parameter w is defined as:

$$\Omega(\boldsymbol{\theta}) = \|\boldsymbol{w}\|_1 = \sum_i |w_i|$$

- We will now discuss the effect of L^1 regularization on the simple linear regression model, with no bias parameters, that we studied in our analysis of L^2 regularization.
- In particular, we are interested in delineating the differences between L^1 and L^2 forms of regularization.

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- As with L^2 weight decay, L^1 weight decay controls the strength of the regularization by scaling the penalty Ω using a positive hyperparameter α.
- Thus, the regularized objective function $\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$ is given by

$$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \alpha \|\boldsymbol{w}\|_1 + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$$

  with the corresponding gradient:

$$\nabla_{\boldsymbol{w}} \tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \alpha \operatorname{sign}(\boldsymbol{w}) + \nabla_{\boldsymbol{w}} J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$$

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- Out simple linear model has a quadratic cost function that we can represent via its Taylor series.
- Alternately, we could imaging that this is a truncated Taylor series approximating the cost function of a more sophisticated model.
- The gradient in this setting is given by

$$\nabla_w \tilde{J}(w) = \mathsf{H}(w - w^*)$$

- Because the L^1 penalty does not admit clean algebraic expressions in the case of a full general Hessian, we will also make the further simplifying assumption that the Hessian is a diagonal, $\mathsf{H} = \mathrm{diag}([H_{1,1}, \ldots, H_{n,n}])$, where each $H_{i,i} > 0$.
- This assumption holds if the data for the linear regression problem has been preprocessed to remove all correlation between the input features, which may be accomplished using PCA.

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- Because the L^1 penalty does not admit clean algebraic expressions in the case of a full general Hessian, we will also make the further simplifying assumption that the Hessian is a diagonal, $\mathbf{H} = \mathrm{diag}([H_{1,1}, \ldots, H_{n,n}])$, where each $H_{i,i} > 0$.
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- Our quadratic approximation of the L^1 regularized objective function decomposes into a sum over the parameters:

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- The problem of minimizing this approximate cost function has an analytical solution (for each dimension i), with the following form:

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    1. The case where $w_i^* \leq \frac{\alpha}{H_{i,i}}$. Here the optimal value of w_i under the regularized objective is simply $w_i = 0$. This occurs because the contribution of $J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$ to the regularized objective $\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$ is overwhelmed–in direction i–by the L^1 regularization which pushes the value of w_i to zero.
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- In comparison to L^2 regularization, L^1 regularization results in a solution that is more *sparse*.
- Sparsity in this context refers to the fact that some parameters have an optimal value of zero.
- The sparsity property induced by L^1 regularization has been used extensively as a *feature selection* mechanism.
- Feature selection simplifies a machine learning problem by choosing which subset of the available features should be used.
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Sparsity? L^1 and L^2

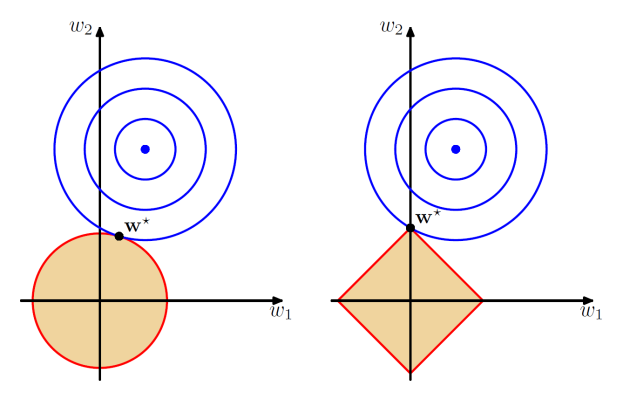

Fig. 2: Plot of the contours of the unregularized error function (blue) along with the constraint region for the quadratic regularizer on the left and the lasso regularizer on the right.

Norm Penalties as Constrained Optimization

- Consider the cost function regularized by a parameter norm penalty:

$$\tilde{J}(\boldsymbol{\theta}; X, y) = J(\boldsymbol{\theta}; X, y) + \alpha\Omega(\boldsymbol{\theta})$$

- If we want to constrain $\Omega(\boldsymbol{\theta})$ to be less than some constant k, we could construct a generalized Language function

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\alpha}; X, y) = J(\boldsymbol{\theta}; X, y) + \alpha(\Omega(\theta) - k)$$

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Regularization and Under-Constrained Problems

- In some cases, regularization is necessary.
- Many linear models in machine learning, including linear regression and PCA, depend on inverting the matrix $X^T X$.
- This is not possible whenever $X^T X$ is singular.
- This matrix can be singular whenever the data generating distribution truly has no variance in some direction, or when no variance in **observed** in some direction because there are fewer examples (rows of X) than input features (columns of X).
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- These linear problems have closed form solutions when the relevant matrix is invertible.
- It is also possible for a problem with no closed form solution to be underdetermined.
- An example is logistic regression applied to a problem where the classes are linearly separable.
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- We can solve underdetermined linear equations using the Moore-Penrose pseudoinverse. Recall that one definition of the pseudoinverse X^+ of a matrix X is

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Dataset Augmentation

- The best way to make a machine learning model generalize better is to train it on more data.
- In practice, it is limited.
- Create fake data and add it to the training set.
- This approach is easiest for classification.
- A classifier needs to take a complicated, high dimensional input x and summarize it with a single category identity y.
- This means that the main task facing a classifier is to be invariant to a wide variety of transformations.
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- One way to improve the robustness of neural networks is simply to train them with random noise applied to their inputs.
- Input noise injection is part of some unsupervised learning algorithms such as the denoising autoencoder (Vincent et al. [2008]).
- Dropout, a powerful regularization strategy can be seen as a process of constructing new inputs by **multiplying** by noise.

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- For some models, the addition of noise with infinitesimal variance at the input of the model is equivalent to imposing a penalty on the norm of the weights (Bishop [1995b,a]).
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- Noise applied to the hidden units is such an important topic; the dropout algorithm describe later.
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- We study the regression setting, where we wish to train a function $\tilde{y}(\boldsymbol{x})$ that maps a set of features $\boldsymbol{x}$ to a scalar using the least-squares cost function between the model predictions $\tilde{y}(\boldsymbol{x})$ and the true values y:

$$J = \mathbb{E}_{p(x,y)}\left[(\hat{y}(x) - y)^2\right]$$

- The training set with m examples: $(\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(m)}, y^{(m)})$.
- We now assume that with each input presentation we also include a random perturbation $\epsilon_W \mathcal{N}(\epsilon; \boldsymbol{0}, \eta I)$ of the network weights.
- We denote the perturbed model as $\hat{y}_{\epsilon_W}(\boldsymbol{x})$. The objective function thus becomes:

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- In the paradigm of semi-supervised learning, both unlabeled examples from $P(x)$ and labeled examples from $P(x, y)$ are used to estimate $P(y|x)$ or predict y from x.
- In the context of deep learning, semi-supervised learning usually refers to learning a representation $h = f(x)$. The goal is to learn a representation so that **examples from the same class have similar representations**.
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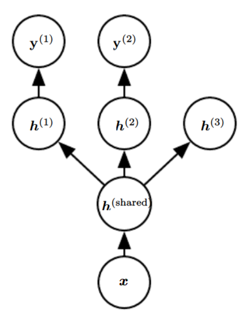
Multi-Task Learning

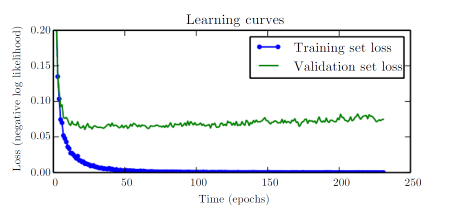
- Here is a very common form of multi-task learning.
- Different supervised tasks (predicting $y^{(i)}$ given x) share the same input x, as well as some intermediate-level representation $h^{(\text{shared})}$ capturing a common pool of factors.
- The model has two kinds of parts:
  1. Task-specific parameters (which only benefit from the examples of their task to achieve good generalization). These are the upper layers.
  2. Generic parameters, shared across all the tasks (which benefit from the pooled data of all the tasks). These are the lower years.



- The factors that explain the variations are shared across two or more tasks.

Early Stopping

- When training large models with sufficient representational capacity to overfit the task, we often observe that training error decreases steadily over time, but validation set error begins to rise again.



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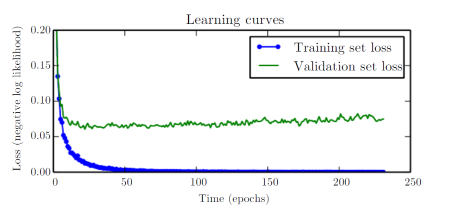

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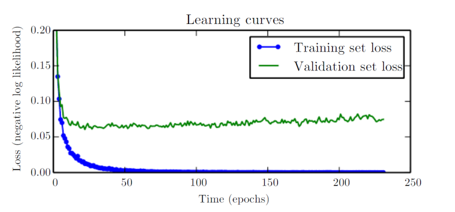

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Let n be the number of steps between evaluations.
Let p be the ”patience”, the number of times to observe worsening validation set error before giving up.
Let $\boldsymbol{\theta}_o$ be the initial parameters.
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}_o$; $i \leftarrow 0$; $j \leftarrow 0$; $v \leftarrow \infty$; $i^* \leftarrow i$
while $j < p$ **do**
    Update $\boldsymbol{\theta}$ by running the training algorithm for n steps.
    $i \leftarrow i + n$; $v' \leftarrow \text{ValidationSetError}(\boldsymbol{\theta})$
    if $v' < v$ **then**
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end while
Best parameters are $\boldsymbol{\theta}^*$, best number of training steps is i^*.

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  else
    $j \leftarrow j + 1$
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end while
Best parameters are $\boldsymbol{\theta}^*$, best number of training steps is i^*.

Early Stopping

Algorithm 4 Early Stopping Algorithm

Let n be the number of steps between evaluations.
Let p be the "patience", the number of times to observe worsening validation set error before giving up.
Let $\boldsymbol{\theta_o}$ be the initial parameters.
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Early Stopping

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Early Stopping

- One way to think of early stopping is as a very efficient hyperparameter selection algorithm.
- In this view, the number of training steps is just another hyperparameter.
- The only significant cost to choosing this hyperparameter automatically via early stopping is running the validation set evaluation periodically during training.
- An additional cost to early stopping is the need to maintain a copy of the best parameters. This cost is generally negligible. (GPU->CPU/MEMORY->HDD).

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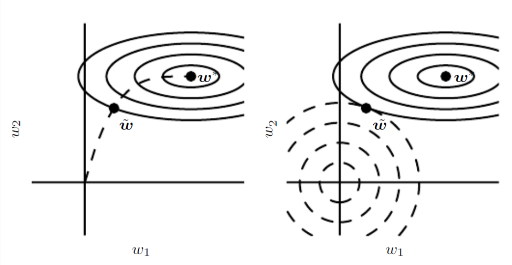
Early Stopping

- How early stopping acts as a regularizer?
- Bishop [1995b] , Sjöberg and Ljung [1995] argued that early stopping has the effect of restricting the optimization procedure to a relatively small volume of parameter space in the neighborhood of the initial parameter value $\boldsymbol{\theta_o}$.



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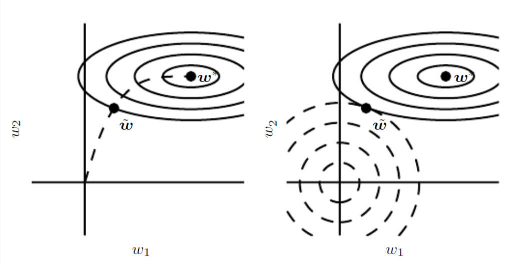

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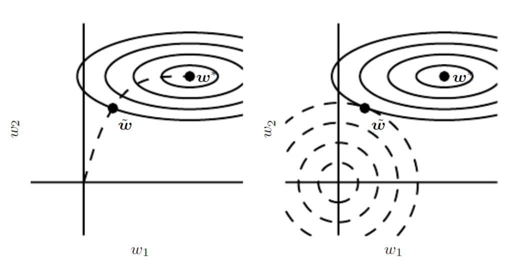

Early Stopping

- In order to compare with classical L^2 regularization, we examine a simple setting where the only parameters are linear weights ($\boldsymbol{\theta} = \boldsymbol{w}$).
- We can model the cost function J with a quadratic approximation in the neighborhood of the empirically optimal value of the weights $\boldsymbol{w}^*$:

$$\hat{J}(\boldsymbol{\theta}) = J(\boldsymbol{w}^*) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}^*)^T \boldsymbol{H}(\boldsymbol{w} - \boldsymbol{w}^*)$$

  where $\boldsymbol{H}$ is Hessian matrix of J with respect to $\boldsymbol{w}$ evaluated at $\boldsymbol{w}^*$.
- Given the assumption that $\boldsymbol{w}^*$ is a minimum of $J(\boldsymbol{w})$, we know that $\boldsymbol{H}$ is positive semidefinite.

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Early Stopping

- Under a local Taylor series approximation, the gradient:

$$\nabla_w \hat{J}(w) = H(w - w^*)$$

- We are going to study the trajectory followed by the parameter vector during training.
- For simplicity, let us set the initial parameter vector to the origin, that is $w^{(0)} = \mathbf{0}$.
- Let us suppose that we update the parameters via gradient descent:

$$\begin{aligned} w^{(\tau)} &= w^{(\tau-1)} - \epsilon \nabla_w J(w^{(\tau-1)}) \\ &= w^{(\tau-1)} - \epsilon H(w^{(\tau-1)} - w^*) \\ w^{(\tau)} - w^* &= (I - \epsilon H)(w^{(\tau-1)} - w^*) \end{aligned}$$

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- Let us now rewrite this expression in the space of the eigenvectors of H, exploiting the eigendecomposition of H : $H = Q\mathbf{\Lambda}Q^T$, where $\mathbf{\Lambda}$ is a diagonal matrix and Q is an orthonormal basis of eigenvectors.

$$\begin{aligned} w^{(\tau)} - w^* &= (I - \epsilon Q\mathbf{\Lambda}Q^T)(w^{(\tau-1)} - w^*) \\ Q^T(w^{(\tau)} - w^*) &= (I - \epsilon\mathbf{\Lambda})Q^T(w^{(\tau-1)} - w^*) \end{aligned}$$

- Assuming that $w^{(0)} = 0$ and that ϵ is chosen to be small enough to guarantee $|1 - \epsilon\lambda_i| < 1$, the parameter trajectory during training training after τ parameter updates is as follows:

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- In L^2 regularization:

$$\tilde{w} = Q(\boldsymbol{\Lambda} + \boldsymbol{\alpha} I)^{-1}\boldsymbol{\Lambda} Q^T w^* \quad (1)$$

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- Then L^2 regularization and early stopping is equivalent.
- Going even further, by taking logarithms and using the series expansion for $\log(1 + x)$, if all λ_i are small then:

$$\tau \approx \frac{1}{\epsilon\alpha} \quad ; \quad \alpha \approx \frac{1}{\tau\epsilon} \quad (4)$$

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Parameter Tying and Parameter Sharing

- Thus far, we have discussed adding constraints or penalties to the parameters.
- However, sometimes we may need other ways to express our prior knowledge about suitable values of the model parameters.
- Sometimes we might not know precisely what values that parameters should take but we know, from knowledge of the domain and model architecture, that there should be some dependencies between the model parameters.
- A common type of dependency that we often want to express is that certain parameters should be close to one another.

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Consider the following scenario:

- We have two models performing the same classification task.
- But with somewhat different input distributions.
- Formally, we have model A with parameters $\boldsymbol{w}^{(A)}$ and model B with parameters $\boldsymbol{w}^{(B)}$.
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- Let us imagine that the tasks are similar enough (perhaps with similar input and output distributions) that we believe the model parameters should be close to each other: $\forall i, w_i^{(A)}$ should be close to $w_i^{(B)}$. We can leverage this information through regularization.
- Specifically, we can use a parameter norm penalty of the form: $\Omega(\boldsymbol{w}^{(A)}, \boldsymbol{w}^{(B)}) = \|\boldsymbol{w}^{(A)} - \boldsymbol{w}^{(B)}\|_2^2$. Here we used an L^2 penalty, but other choices are also possible.

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- This kind of approach was proposed by Lasserre et al. [2006], who regularized the parameters of one model, trained as a classifier in a supervised paradigm, to be close to the parameters of another model, trained in an unsupervised paradigm (to capture the distribution of the observed input data).
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Parameter Tying and Parameter Sharing

- While a parameter norm penalty is one way to regularize parameters to be close to one another, the more popular way is to use constraints: **to force sets of parameters to be equal**.
- This method of regularization is often referred to as *parameter sharing*, where we interpret the various models or model components as sharing a unique set of parameters.
- A significant advantage of parameter sharing over regularizing the parameters to be close (via a norm penalty) is that only a subset of the parameters need to be stored in memory.
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Parameter Tying and Parameter Sharing
Convolutional Neural Networks

- By far the most popular and extensive use of parameter sharing occurs in *convolutional neural networks* (CNNs) applied to computer vision.
- Natural images have many statistical properties that are invariant to translation.
- CNNs take this property into account by sharing parameters across multiple image locations.
- The same feature (a hidden unit with the same weights) is computed over different locations in the input.
- This means that we can find a object with the same object detector whether the object appears at column i or column $i+1$ in the image.
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Sparse Representation

- Weight decay acts by placing a penalty directly on the model parameters.
- Another strategy is to place a penalty on the activations of the units in a neural network, encouraging their activations to be sparse.
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- We have already discussed how L^1 penalization induces a sparse parametrization – meaning that many of the parameters become zero (or close to zero).
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- A simplified view of this distinction can be illustrated in the context of linear regression:

$$\underbrace{\begin{bmatrix} 18 \\ 5 \\ 15 \\ -9 \\ -3 \end{bmatrix}}_{\mathbf{y} \in \mathbb{R}^m} = \underbrace{\begin{bmatrix} 4 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 3 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & -4 \\ 1 & 0 & 0 & 0 & -5 & 0 \end{bmatrix}}_{\mathbf{A} \in \mathbb{R}^{m \times n}} \underbrace{\begin{bmatrix} 2 \\ 3 \\ -2 \\ -5 \\ 1 \\ 4 \end{bmatrix}}_{\mathbf{x} \in \mathbb{R}^n}$$

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- Representational regularization is accomplished by the same sorts of mechanisms that we have used in parameter regularization.
- Norm penalty regularization of representation is performed by adding to the loss function J a norm penalty on the **representation**. This penalty is denoted $\Omega(\boldsymbol{h})$. As before, we denote the regularized loss function by $\tilde{J}$:

$$\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) + \alpha\Omega(\boldsymbol{h})$$

- Just as an L^1 penalty on the parameters induces parameter sparsity, an L^1 penalty on the elements of the representation induces representational sparsity:

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- Of course, the L^1 penalty is only one choice of penalty that can result in a sparse representation.
- Others include the penalty derived from a Student-t prior on the representation (Olshausen and Field [2005], Bergstra et al. [2011]) and KL divergence penalties (Larochelle and Bengio [2008]) that are especially useful for representations with elements constrained to lie on the unit interval.
- Lee et al. [2008] and Goodfellow et al. [2009] both provide examples of strategies based on regularizing the average activation across several examples, $\frac{1}{m}\sum_i \boldsymbol{h}^{(i)}$, to be near some target value, such as a vector with 0.01 for each entry.

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- Other approaches obtain representational sparsity with a hard constraint on the activation values.
- For example, *orthogonal matching pursuit* (Pati et al. [1993]) encodes an input $\boldsymbol{x}$ with representation $\boldsymbol{h}$ that solves the constrained optimization problem

$$\arg\min_{\boldsymbol{h}, \|\boldsymbol{h}\|_0 < k} \|\boldsymbol{x} - \boldsymbol{W}\boldsymbol{h}\|^2$$

  where $\|\boldsymbol{h}\|_0$ is the number of non-zero entries of $\boldsymbol{h}$.
- This problem can be solved efficiently when $\boldsymbol{W}$ is constrained to be orthogonal.
- This method is often called OMP-k with the value of k specified to indicate the number of non-zero features allowed.
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Bagging and Other Ensemble Methods

- Bagging(short for boostrap aggregating) is a technique for reducing generalization error by combining several models (Breiman [1996]).
- The idea is to train several different models separately, then have all of the models vote on the output for test examples.
- Thi is an example of a general strategy in machine learning called *model averaging*.
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- The reason that model averaging works is that different models will usually not make all the same errors on the test set.
- Consider for example a set of k regression models.
- Suppose that each model makes an error ϵ_i on each example, with the errors drawn from a zero-mean multivariate normal distribution with variance $\mathbb{E}[\epsilon_u^2] = v$ and covariance $\mathbb{E}[\epsilon_i \epsilon_j] = c$.
- Then the error made by the average prediction of all the ensemble models is $\frac{1}{k}\sum_i \epsilon_i$.
- The expected squared error of the ensemble predictor is

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- For example, each member of the ensemble could be formed by training a completely different kind of model using a different algorithm or objective function.
- Bagging is a method that allows the same kind of model, training algorithm and objective function to be reused several times.
- Specifically, bagging involves constructing k different datasets.
- Each dataset has the same number of examples as the original dataset, but each dataset is constructed by sampling with replacement from the origin dataset.
- This means that, with high probability, each dataset is missing some of the examples from the original dataset and also contains several duplicate examples.

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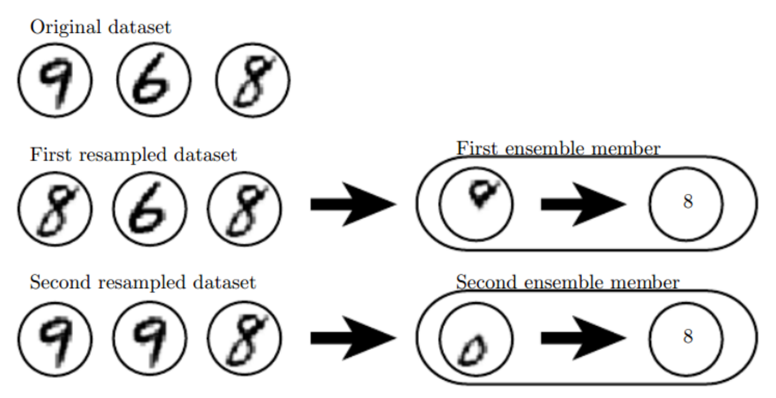

Fig. 3: A cartoon depiction of how bagging works

- Neural networks reach a wide enough variety of solution points that they can often benefit from model averaging even if all of the models are trained on the same dataset.
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Dropout

- Dropout ([Srivastava et al., 2014]) provides a computationally inexpensive but powerful method of regularizing a broad family of models.
- Dropout can be thought of as a method of making bagging practical for ensembles of very many large neural networks.
- Bagging involves training multiple models, and evaluating multiple models on each test example.
- This seems impractical when each model is a large neural network, since training and evaluating such networks is costly in terms of runtime and memory.
- It is common to use ensembles of five to ten neural networks. but more than this rapidly becomes unwieldy.
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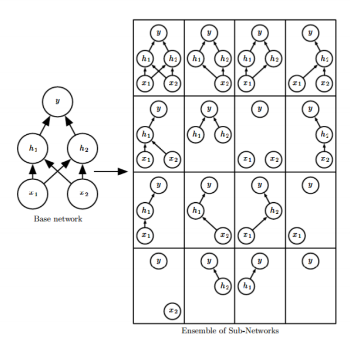
Dropout

Specifically, dropout trains the ensemble consisting of all sub-networks that can be formed by removing non-output units from an underlying base network.

- In the most modern neural networks, based on a series of affine transformations and nonlinearities, we can effectively remove a unit from a network by multiplying its output value by zero.
- This procedure requires some slight modification for models such as radial basis function networks, which take the difference between the unit's state and some reference value.



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- Here, we present the dropout algorithm in terms of multiplication by zero for simplicity, but it can be trivially modified to work with other operations that remove a unit from the network.
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- Specifically, to train with dropout, we use a minibatch-based learning algorithm that makes small steps, such as stochastic gradient descent.
- Each time we load an example into a minibatch, we randomly sample a different binary mask to apply to all of the input and hidden units in the network.
- The mask for each unit is sampled independently from all of the others.
- The probability of sampling a mask value of one is a hyperparameter fixed before training begins.
- Typically, an input unit is included with probability 0.8 and a hidden unit is included with probability 0.5.
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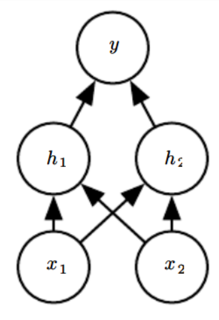

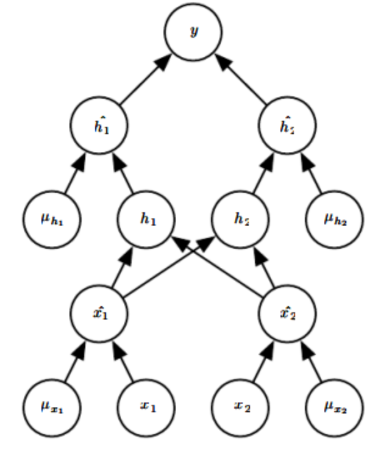

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