Deep Learning Book

Chapter 7
Regularization for Deep Learning

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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? (Generalization)
- 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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- 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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- 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**.
- Instead, 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:

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Recall: Quadratic Approximation

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- 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 $\hat{J}(\theta)$, 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 $\hat{J}$.
- We use the variable $\tilde{w}$ to represent the location of the minimum.

$$\alpha \tilde{w} + \mathsf{H}(\tilde{w} - w^*) = 0$$

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

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

- 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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- We see that the effect of weight decay is to rescale w^* along the axes defined by the eigenvectors of H.
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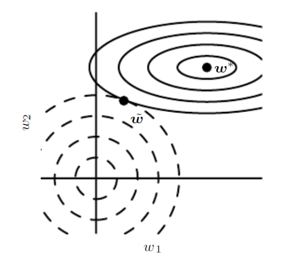
This effect is illustrated in figure:

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



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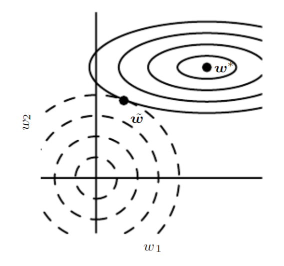

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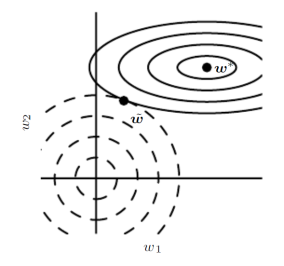

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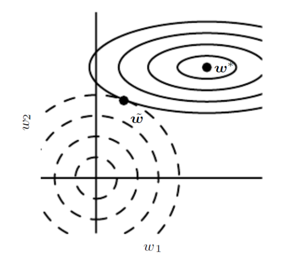

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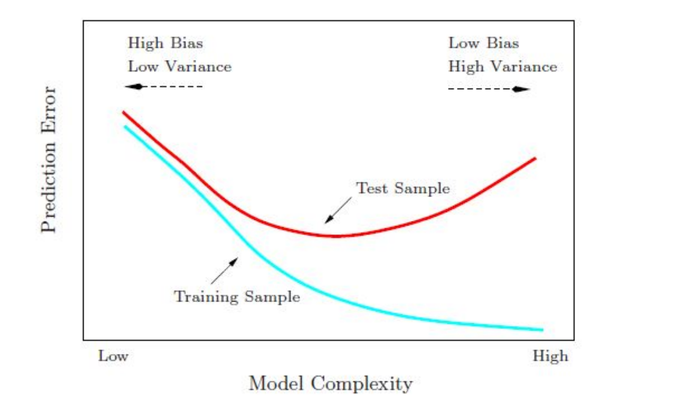

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- How do these effects relate to machine learning in particular?
- We can find out by studying linear regression, the cost function is the sum of squared errors:

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

- 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.
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L^1 Regularization

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L^1 Regularization

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

- From this equation, we can see that the effect of L^1 regularization is quite different from that of L^2 regularization.
- We can see that the regularization contribution to the gradient no longer scales linearly with each w_i; instead it is a constant factor with a sign equal to $\mathrm{sign}(w_i)$.
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L^1 Regularization

- 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

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

- 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, $\mathbf{H} = \mathrm{diag}([H_{1,1}, \dots, H_{n,n}])$, 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:

$$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{w}^*; \boldsymbol{X}, \boldsymbol{y}) + \sum_i \left[\frac{1}{2} H_{i,i} (\boldsymbol{w}_i - \boldsymbol{w}_i^*)^2 + \alpha \left| w_i \right| \right]$$

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

$$w_i = \mathrm{sign}(w_i^*) max \left\{ |w_i^*| - \frac{\alpha}{H_{i,i}}, 0 \right\}$$

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- Consider the situation where $w_i^* > 0$ for all i. There are two possible outcomes:
  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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L^1 Regularization

- 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.
- In particular, the well known LASSO ([Tibshirani, 1996]) (least absolute shrinkage and selection operator) model integrates an L^1 penalty with a linear model and a least squares cost function.

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Sparsity? L^1 and L^2

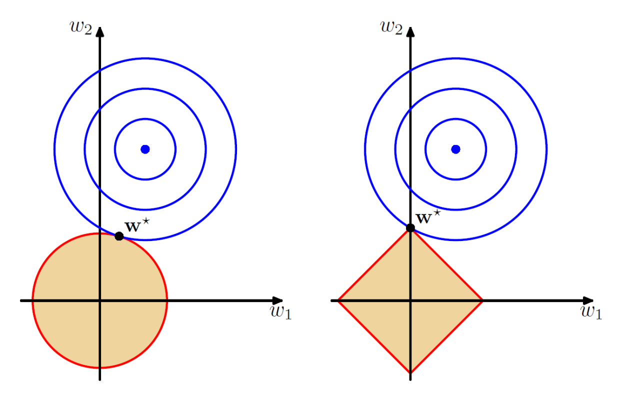

Fig. 2: Plot of the contours of the unregularized error function (blue) along with the constraint region for the quadratic regularizer on the left and the lasso regularizer on the right.

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 Lagrange function

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

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$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \max_{\alpha, \alpha \geq 0} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\alpha})$$

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- Many different procedures are possible–some may use gradient descent, while others may use analytical solutions for where the gradient is zero–but in all procedures α must increase whenever $\Omega(\boldsymbol{\theta}) > k$ and decrease whenever $\Omega(\boldsymbol{\theta}) < k$.
- All positive α encourage $\Omega(\boldsymbol{\theta})$ to shrink.
- The optimal value a^* will encourage $\Omega(\theta)$ to shrink, but not so strongly to make $\Omega(\boldsymbol{\theta})$ become less than k.

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- To gain some insight into the effect of the constraint, we can fix α^* and view the problem as just a function of θ:

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- We can thus think of a parameter norm penalty as imposing a constraint on the weights.
- If Ω is the L^2 norm, then the weights are constrained to lie in an L^2 ball.
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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).
- In this case, many forms of regularization correspond to inverting $X^T X + \alpha I$ instead. This regularized matrix is guaranteed to be invertible.

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- In this case, many forms of regularization correspond to inverting $X^TX + \alpha I$ instead. This regularized matrix is guaranteed to be invertible.

Regularization and Under-Constrained Problems

- 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.
- If a weight vector w is able to achieve perfect classification, then $2w$ will also achieve perfect classification and higher likelihood.
- An iterative optimization procedure like SGD will continually increase the magnitude of w and, in theory, will never halt.
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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

$$X^+ = \lim_{a \to 0} (X^T X + \alpha I)^{-1} X^T$$

- We can now recognize this equation as performing linear regression with weight decay.
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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, the amount of data we have 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.
- We can generate new (x, y) pairs easily just by transforming the x inputs in our training set.

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- Dataset augmentation is effective for speech recognition task as well (Jaitly and Hinton [2013]).
- Inject noise in the input to a neural network can also be seen as a form of data augmentation (Sietsma and Dow [1991]).
- For many classification and even some regression tasks, the task should still be possible to solve even if small random noise is added to the input.
- One way to improve the robustness of neural networks is simply to train them with random noise applied to their inputs.
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Noise Robustness

- 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]).
- Noise injection can be much more powerful than simply shrinking the parameters, especially when the noise is added to the hidden units.
- Noise applied to the hidden units is such an important topic; the dropout algorithm describe later.
- Another way that noise can be added into the weights.
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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: $(\boldsymbol{x}^{(1)}, y^{(1)}), \dots, (\boldsymbol{x}^{(m)}, y^{(m)})$.
- We now assume that with each input presentation we also include a random perturbation $\epsilon_W \mathcal{N}(\epsilon; \mathbf{0}, \eta I)$ of the network weights.
- We denote the perturbed model as $\hat{y}_{\epsilon_W}(x)$. The objective function thus becomes:

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Injecting Noise at the Output Target

- Most datasets have some amount of mistakes in the y labels.
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- In the paradigm of semi-supervised learning, both unlabeled examples from $P(\mathbf{x})$ and labeled examples from $P(\mathbf{x}, \mathbf{y})$ are used to estimate $P(\mathbf{y}|\mathbf{x})$ or predict $\mathbf{y}$ from $\mathbf{x}$.
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Semi-Supervised Learning

- One can construct models in which a generative model of either (x) or $P(x, y)$ shares parameters with a discriminative model of $P(y|x)$.
- The generative criterion then express a particular form of prior belief about the solution to the supervised learning problem, namely that the structure of $P(x)$ is connected to the structure of $P(y|x)$ in a way that is captured by the shared parameterization.
- By controlling how much of the generative criterion is included in the total criterion, one can find a better trade-off than with a purely generative or purely discriminative training criterion.
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Multi-Task Learning

- Multi-task learning is a way to improve generalization by pooling the examples arising out of several tasks.
- In the same way that additional training examples put more pressure on the parameters of the model towards values that generalize well, when part of a model is shared across tasks, model often yield better generalization.

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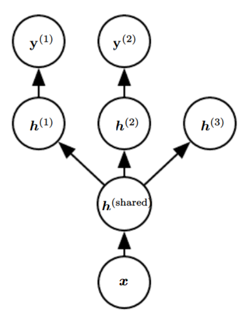
Multi-Task Learning

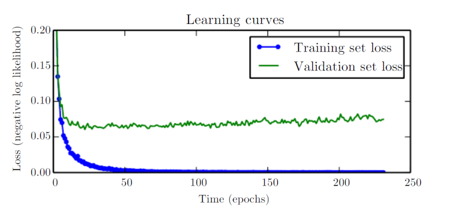
- Here is a very common form of multi-task learning.
- Different supervised tasks (predicting $y^{(i)}$ given x) share the same input x, as well as some intermediate-level representation $h^{(\text{shared})}$ capturing a common pool of factors.
- The model has two kinds of parts:
  1. Task-specific parameters (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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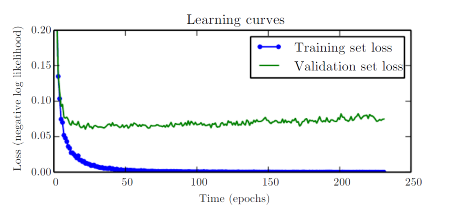

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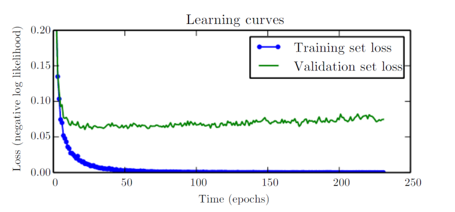

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Algorithm 1 Early Stopping Algorithm

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.
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta_o}$; $i \leftarrow 0$; $j \leftarrow 0$; $v \leftarrow \infty$; $i^* \leftarrow i$
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**
    $j \leftarrow 0$; $\boldsymbol{\theta}^* \leftarrow \boldsymbol{\theta}$; $i^* \leftarrow i$; $v \leftarrow v'$
  else
    $j \leftarrow j + 1$
  end if
end while
Best parameters are $\boldsymbol{\theta}^*$, best number of training steps is i^*.

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Algorithm 2 Early Stopping Algorithm

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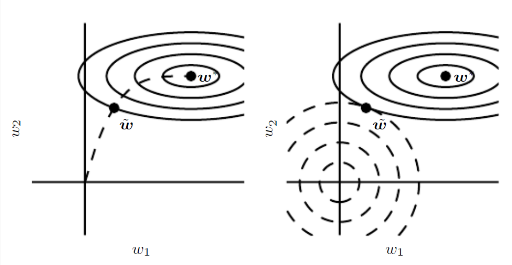
- How early stopping acts as a regularizer?
- Bishop [1995b] , Sjöberg and Ljung [1995] argued that early stopping has the effect of restricting the optimization procedure to a relatively small volume of parameter space in the neighborhood of the initial parameter value $\boldsymbol{\theta_o}$.



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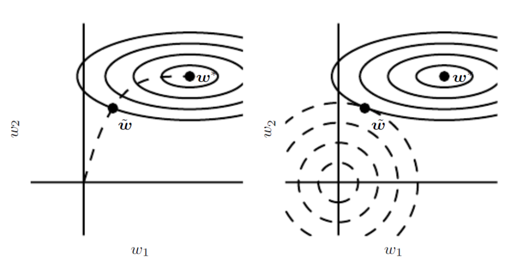

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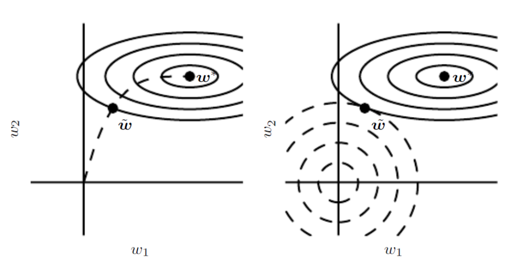

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- In order to compare with classical L^2 regularization, we examine a simple setting where the only parameters are linear weights ($\boldsymbol{\theta} = \boldsymbol{w}$).
- We can model the cost function J with a quadratic approximation in the neighborhood 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 $\boldsymbol{w}^*$.
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- 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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$$\begin{aligned} w^{(\tau)} - w^* &= (I - \epsilon Q\mathbf{\Lambda}Q^T)(w^{(\tau-1)} - w^*) \\ Q^T(w^{(\tau)} - w^*) &= (I - \epsilon\mathbf{\Lambda})Q^T(w^{(\tau-1)} - w^*) \end{aligned}$$

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- Compare with $Q^T w^{(\tau)} = [I - (I - \epsilon\Lambda)^\tau] Q^T w^*$, we can find:

$$(I - \epsilon\Lambda)^\tau = (\Lambda + \alpha I)^{-1} \alpha$$

- 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:

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

- That is, under these assumptions, the number of training iterations τ plays a role inversely proportional to the L^2 regularization parameter, and the inverse of $\tau\epsilon$ plays the role of the weight decay coefficient.

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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.
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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 $\boldsymbol{w}^{(B)}$.
- The two models map the input to different, but related outputs: $\hat{y}^{(A)} = f(\boldsymbol{w}^{(A)}, \boldsymbol{x})$ and $\hat{y}^{(B)} = g(\boldsymbol{w}^{(B)}, \boldsymbol{x})$.

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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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- 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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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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- 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:

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

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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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Sparse Representation

- 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.
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- The idea is to train several different models separately, then have all of the models vote on the output for test examples.
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Bagging and Other Ensemble Methods

- 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

$$\mathbb{E}\left[\left(\frac{1}{k}\sum_i \epsilon_i\right)^2\right] = \frac{1}{k^2}\mathbb{E}\left[\sum_i \left(\epsilon_i^2 + \sum_{i \neq j} \epsilon_i \epsilon_j\right)\right] = \frac{1}{k}v + \frac{k-1}{k}c$$

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Bagging and Other Ensemble Methods

- Different ensemble methods construct the ensemble of the models in different ways.
- 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.
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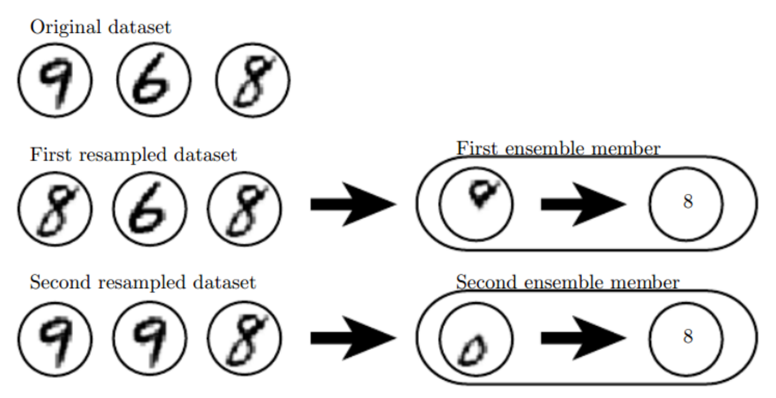

Fig. 3: A cartoon depiction of how bagging works

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- Its use is usually discouraged when benchmarking algorithms for scientific papers.
- Machine learning contest are usually won by methods using model averaging over dozens of models.
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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.
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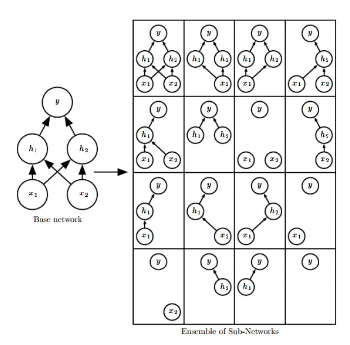
Specifically, dropout trains the ensemble consisting of all sub-networks that can be formed by removing non-output units from an underlying base network.

- 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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- 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.
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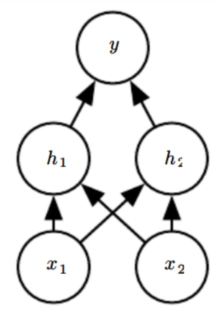

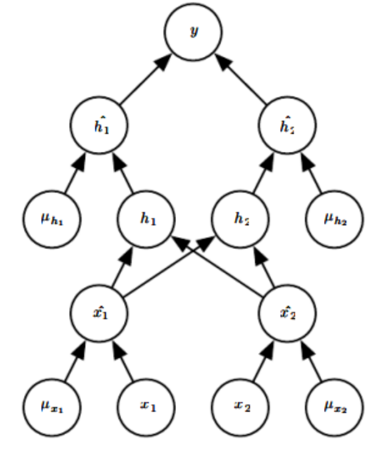

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- To make a prediction, a bagged ensemble must accumulate votes from all of its members. We refer to this process as *inference* in this context.
- Now, we assume that the model's role is to output a probability distribution.
- In the case of bagging, each model i produces a probability distribution $p^{(i)}(y|\mathbf{x})$.
- The prediction of the ensemble is given by the arithmetic mean of all of these distributions

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  where $p(\boldsymbol{\mu})$ is the probability distribution that was used to sample μ at training time.
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- The geometric mean of multiple probability distributions is not guaranteed to be a probability distribution.
- To guarantee that the result is a probability distribution, we impose the requirement that none of the sub-models assigns probability 0 to any event, and we renormalize the resulting distribution.
- The unnormalized probability distribution defined directly by the geometric mean is given by

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- Here we use a uniform distribution over $\boldsymbol{\mu}$ to simplify the presentation, but non-uniform distributions are also possible.
- To make predictions we must re-normalize the ensemble:

$$p_{\text{ensemble}}(y|\mathbf{x}) = \frac{\tilde{p}_{\text{ensemble}}(y|\mathbf{x})}{\sum_{y'} \tilde{p}_{\text{ensemble}}(y'|\mathbf{x})}$$

- The key insight (Hinton et al. [2012]) involved in dropout is that we can approximate p_{ensemble} by evaluating $p(y|\mathbf{x})$ in one model: the model with all units, but with the weight going out of unit i multiplied by the probability of including unit i.
- We call this approach the *weight scaling inference rule*.
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- Because we usually use an inclusion probability of $\frac{1}{2}$, the weight scaling rule usually amounts to dividing the weights by 2 at the end of training, and then using the model as usual.
- Another way to achieve the same result is to multiply the states of the units by 2 during training.
- Either way, the goal is to make sure that the expected total input to a unit at test time is roughly the same as the expected total input to that unit at train time, even though half the units at train time are missing on average.

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- For many classes of models that do not have nonlinear hidden units, the weight scaling inference rule is exact.
- For a simple example, consider a softmax regression classifier with n input variables represented by the vector $\mathbf{v}$:

$$P(\mathrm{y} = y|\mathbf{v}) = \mathrm{softmax}(\mathbf{W}^T\mathbf{v} + b)_y$$

- We can index into the family of sub-models by element-wise multiplication of the input with a binary vector d:

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- The ensemble predictor is defined by re-normalizing the geometric mean over all ensemble members' predictions

$$P_{\text{ensemble}}(\mathrm{y} = y|\mathbf{v}) = \frac{\tilde{P}_{\text{ensemble}}(\mathrm{y} = y|\mathbf{v})}{\sum_{y'} \tilde{P}_{\text{ensemble}}(\mathrm{y} = y'|\boldsymbol{v})}$$

where

$$\tilde{P}_{\text{ensemble}}(\mathrm{y} = y|\boldsymbol{v}) = \sqrt[2^n]{\prod_{\boldsymbol{d} \in \{0,1\}^n} P(\mathrm{y} = y|\mathbf{v}; \boldsymbol{d})}$$

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\tilde{P}_{\text{ensemble}}(\mathrm{y} = y|\mathbf{v}) &= \sqrt[2^n]{\prod_{d\in\{0,1\}^n} P(\mathrm{y} = y|\mathbf{v}; d)} \\
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- The weight scaling rule is also exact in other settings, including regression networks with conditionally normal outputs, and deep networks that have hidden layers without nonlinearities.
- However, the weight scaling rule is only a approximation for deep models that have nonlinearities.
- Though the approximation has not been theoretically characterized, it often works well, empirically.
- Goodfellow et al. [2013b] found experimentally that the weight scaling approximation can work better (in terms of classification accuracy) than Monte Carlo approximations to the ensemble predictor.
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- Gal and Ghahramani [2015] found that some models obtain better classification accuracy using twenty samples and the Monte Carlo approximation. It appears that the optimal choice of inference approximation is problem-depend.
- Srivastava et al. [2014] showed that dropout is more effective than other standard computationally inexpensive regularizers, such as weight decay, filter norm constraints and sparse activity regularization.
- One advantage of dropout is that it is very computationally cheap.
- Another significant advantage of dropout is that it does not significantly limit the type of model or training procedure that can be used.
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- The magnitude of each feature's weight decay coefficient is determined by its variance.
- Similar results hold for other linear models.
- For deep models, dropout is not equivalent to weight decay.

Dropout

- The power of dropout arises from the fact that the masking noise is applied to the hidden units.
- This can be seen as a form of highly intelligent, adaptive destruction of the information content of the input rather than destruction of the raw values of the input.
- For example, if the model learns a hidden unit h_i that detects a face by finding the nose, then dropping h_i corresponds to erasing the information that there is a nose in the image.
- The model must learn another h_i, either that redundantly encodes the presence of a nose, or that detects the face by another feature, such as the mouth.
- Destroying extracted features rather than original values allows the destruction process to make use of all of the knowledge about the input distribution that the model has acquired so far.

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Adversarial Training

- Im many cases, neural networks have begun to reach human performance when evaluated on an i.i.d. test set. It is natural therefore to wonder whether these models have obtained a true human-level understanding of these tasks.
- In order to probe the level of understanding a network has of the underlying task, we can search for examples that the models misclassifies.
- Szegedy et al. [2013] found that even neural networks that perform at human level accuracy have a nearly 100% error rate on examples that are intentionally constructed by using an optimization procedure to search for an input x' near a data point x such that the model output is very different at x'
- In many cases, x' can be so similar to x' that a human observer cannot tell the difference between the original example and the *adversarial example*, but the network can make highly different predictions.

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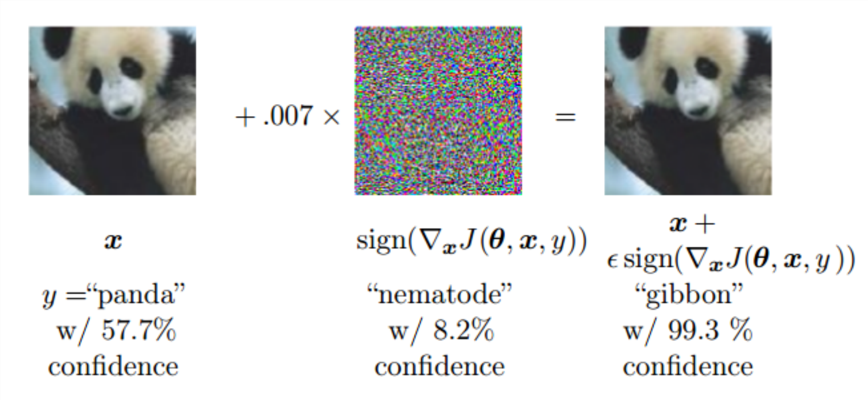

Adversarial Training

- Adversarial examples are interesting in the context of regularization because one can reduce the error rate on the original i.i.d. test set via *adversarial training*– training on adversarially perturbed examples from from the training set.
- Goodfellow et al. [2013a] showed that one of the primary causes of these adversarial examples is excessive linearity.
- Neural networks are built out of primarily linear building blocks.
- In some experiments the overall function they implement proves to be highly linear as a result.
- Unfortunately, the value of a linear function can change very rapidly if it has numerous inputs.
- If we change each input by ϵ, then a linear function with weights w can change by as much as $\epsilon||w||_1$, which can be a very large amount if w is high-dimensional.

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- Adversarial training helps to illustrate the power of using a large function family in combination with aggressive regularization.
- Purely linear models, like logistic regression, are not able to resist adversarial examples because they are forced to be linear.
- Neural networks are able to represent functions that can range from nearly linear to nearly locally constant and thus have the flexibility to capture linear trends in the training data while still learning to resist local perturbation.

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Adversarial Training

- Adversarial examples also provide a means of accomplishing semi-supervised learning.
- At a point $\boldsymbol{x}$ that is not associated with a label in the dataset, the model itself assigns some label $\hat{y}$.
- The model's label $\hat{y}$ may not be the true label, but if the model is high quality, then $\hat{y}$ has a high probability of providing the true label.
- We can seek an adversarial example $\boldsymbol{x}'$ that causes the classifier to output a label y' with $y' \neq \hat{y}$.
- The classifier may then be trained to assign the same label to $\boldsymbol{x}$ and $\boldsymbol{x}'$.
- Adversarial examples generated using not the true label but a label provided by a trained model are called *virtual adversarial examples*.
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Tangent Distance, Tangent Prop, and Manifold Tangent Classifier

- The *tangent prop* algorithm (Simard et al. [1991]) trains a neural net classifier with an extra penalty to make each output $f(\boldsymbol{x})$ of the neural net locally invariant to known factors of variation.
- The directional derivative of f at $\boldsymbol{x}$ in the directions $\boldsymbol{v}^{(i)}$ be small by adding a regularization penalty Ω:

$$\Omega(f) = \sum_i \left((\nabla_x f(x))^2 \, v^{(i)} \right)^2$$

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