CSC413: Homework 3

Tianyu Du (1003801647)

2020/02/29 at 15:57:54

1 Weight Decay

1.1 Under-parameterized Model [0pt]

Solution. Given

$$\mathcal{J}(\hat{\mathbf{w}}) = \frac{1}{2n}\|X\hat{\mathbf{w}} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\hat{\mathbf{w}}^T\hat{\mathbf{w}} \tag{1.1}$$
$$\mathcal{J}(\hat{\mathbf{w}}) = \frac{1}{2n}\|X\hat{\mathbf{w}} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}||\hat{\mathbf{w}}||_2^2 \tag{1.2}$$

The gradient descent converges when $\frac{d}{d\hat{\mathbf{w}}}\mathcal{J}(\hat{\mathbf{w}}) = 0$. Altogether with the fact that $\frac{d}{d\mathbf{x}}||\mathbf{x}||_2^2 = 2\mathbf{x}^T$, the training converges if and only if:

$$\frac{d}{d\hat{\mathbf{w}}}\mathcal{J}(\hat{\mathbf{w}}) = \frac{1}{n}(X\hat{\mathbf{w}} - \mathbf{t})^T X + \lambda\hat{\mathbf{w}}^T \tag{1.3}$$
$$= \frac{1}{n}\hat{\mathbf{w}}^T X^T X - \frac{1}{n}\mathbf{t}^T X + \lambda\hat{\mathbf{w}}^T = 0 \quad (\dagger) \tag{1.4}$$

Note that when $d \leq n$, $rank(X) = d$ implies $X^T X$ is invertible. Suppose $X^T X + n\lambda I$ is invertible as well. Therefore,

$$(\dagger) \implies \left(\hat{\mathbf{w}}^T X^T X + n\lambda\hat{\mathbf{w}}^T\right) = \mathbf{t}^T X \tag{1.5}$$
$$\implies \hat{\mathbf{w}}^T\left(X^T X + n\lambda I\right) = \mathbf{t}^T X \tag{1.6}$$
$$\implies \hat{\mathbf{w}}^T = \mathbf{t}^T X\left(X^T X + n\lambda I\right)^{-1} \tag{1.7}$$
$$\implies \hat{\mathbf{w}} = \left(X^T X + n\lambda I\right)^{-1} X^T\mathbf{t} \tag{1.8}$$

■

1.2 Over-parameterized Model

1.2.1 Warmup: Visualizing Weight Decay [1pt]

Solution. Given

$$\mathbf{x}_1 = (2, 1) \text{ and } t_1 = 2. \tag{1.9}$$

From previous homework, the solution of gradient descent without regularization is

$$\mathbf{w}^* = \left(\frac{4}{5}, \frac{2}{5}\right) \tag{1.10}$$

From the previous part, the gradient descent converges if and only if

$$\begin{align} \frac{d}{d\hat{\mathbf{w}}}\mathcal{J}(\hat{\mathbf{w}}) &= \frac{1}{n}(X\hat{\mathbf{w}} - \mathbf{t})^T X + \lambda \hat{\mathbf{w}}^T \tag{1.11} \\ &= ((2,1)\cdot(w_1, w_2) - 2)(2,1) + \lambda(w_1, w_2) \tag{1.12} \\ &= (2w_1 + w_2 - 2)(2,1) + (\lambda w_1, \lambda w_2) = 0 \tag{1.13} \\ & \tag{1.14} \end{align}$$

Therefore, the solution to gradient descent with weight decay is:

$$\begin{cases} 4w_1 + 2w_2 - 4 + \lambda w_1 & = 0 \\ 2w_1 + w_2 - 2 + \lambda w_2 & = 0 \end{cases} \tag{1.15}$$

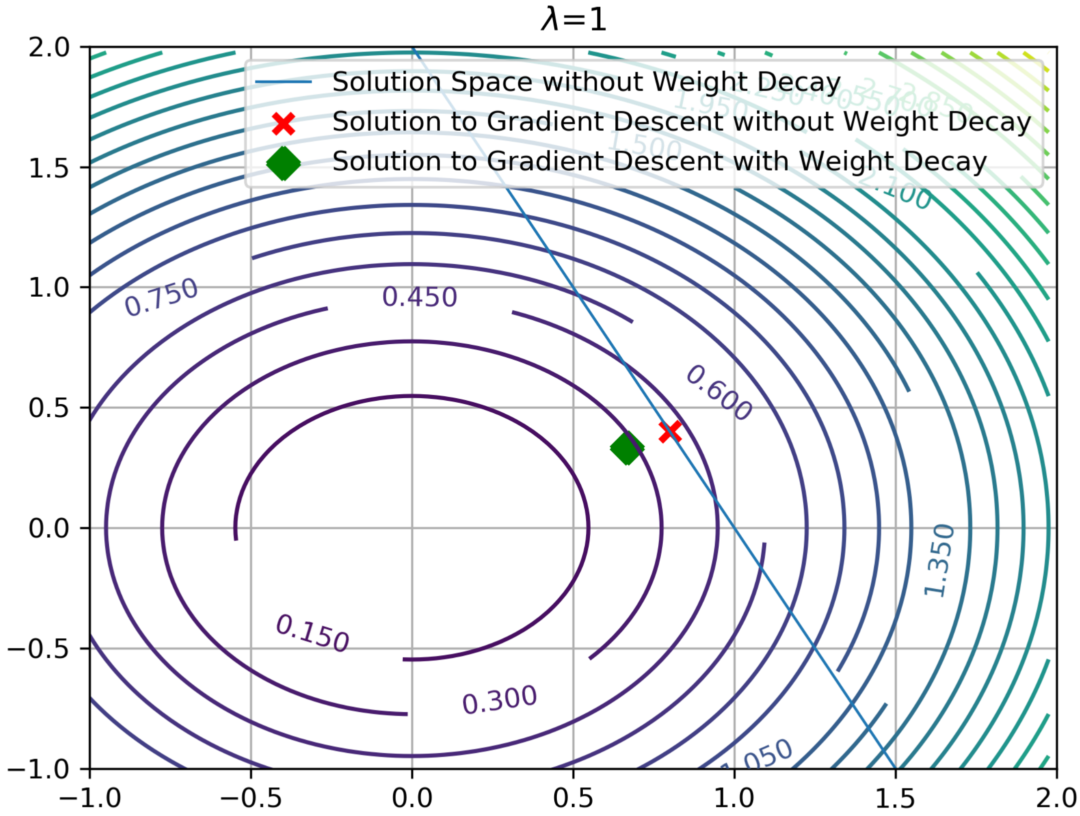
$$\implies \begin{cases} w_1^* & = \frac{4}{\lambda+5} \\ w_2^* & = \frac{2}{\lambda+5} \end{cases} \tag{1.16}$$

The solution space is parameterized by λ as following

$$\mathcal{S} := \left\{ \frac{4}{\lambda+5}, \frac{2}{\lambda+5} : \lambda \in \mathbb{R}_+ \right\} \tag{1.17}$$

which is a singleton uniquely determined by λ. Note that the following visualization assumes $\lambda = 1$.

Figure 1.1: Visualization



■

1.2.2 Gradient Descent and Weight Decay [0pt]

Solution. The solution to gradient descent with weight decay has been derived in the previous section:

$$\mathbf{w}^*_{\text{weight decay}} = \left(\frac{4}{\lambda+5}, \frac{2}{\lambda+5}\right) \tag{1.18}$$

■

1.3 Adaptive optimizer and Weight Decay [1pt]

2 Ensembles and Bias-variance Decomposition

2.1 Weight Average or Prediction Average?

2.1.1 [1pt]

Solution. Without loss of generality, assume the bias is zero. This is equivalent to inserting a column of ones to the X, so that $X \in \mathbb{R}^{n\times(d+1)}$, and we can ignore the bias. ■

3 Generalization and Dropout

3.1 Regression Coefficients

3.1.1 Regression from X_1 [0pt]

Solution. ■

3.1.2 Regression from X_2 [1pt]

Solution. Since we are using X_2 only, equivalently, we can set the weight of X_1 to zero:

$$\begin{aligned}
\mathcal{J} &= \mathbb{E}_{(x_2,y)\sim(X_2,Y)}[(y-\hat{y})^2] && (3.1)\\
&= \mathbb{E}_{(x_2,y)\sim(X_2,Y)}[(y-w_2x_2)^2] && (3.2)\\
&= \mathbb{E}_{(x_2,y)\sim(X_2,Y)}[(y-w_2(y+Gaussian(0,1)))^2] && (3.3)\\
&= \mathbb{E}_{(x_2,y)\sim(X_2,Y)}[((1-w_2)y-w_2Gaussian(0,1))^2] && (3.4)\\
&= \mathbb{E}_{(x_2,y)\sim(X_2,Y)}[((1-w_2)y)^2]+w_2^2\mathbb{E}_{(x_2,y)\sim(X_2,Y)}[Gaussian(0,1)^2] && (3.5)\\
&= (1-w_2)^2\mathbb{E}_{y\sim Y}[y^2]+w_2^2 && (3.6)
\end{aligned}$$

Taking the gradient and solve the first order condition:

$$\begin{aligned}
&\nabla_{w_2}(1-w_2)^2\mathbb{E}_{y\sim Y}[y^2]+w_2^2 = 0 && (3.7)\\
&\implies -2(1-w_2)\mathbb{E}_{y\sim Y}[y^2]+2w_2 = 0 && (3.8)\\
&\implies \mathbb{E}_{y\sim Y}[y^2]-w_2\mathbb{E}_{y\sim Y}[y^2]-w_2 = 0 && (3.9)\\
&\implies \mathbb{E}_{y\sim Y}[y^2]+w_2(1-\mathbb{E}_{y\sim Y}[y^2]) = 0 && (3.10)\\
&\implies w_2 = \frac{\mathbb{E}_{y\sim Y}[y^2]}{\mathbb{E}_{y\sim Y}[y^2]+1} && (3.11)
\end{aligned}$$

The expectation of y^2 is

$$\begin{aligned}
\mathbb{E}_{y\sim Y}[y^2] &= \mathbb{E}_{x_1\sim X_1}(x_1+Gaussian(0,\sigma^2))^2 && (3.12)\\
&= 2\sigma^2 && (3.13)\\
\implies w_2 &= \frac{2\sigma^2}{2\sigma^2+1} && (3.14)
\end{aligned}$$

■

3.1.3 Regression from (X_1, X_2) [1pt]

4 Hard-Coding Recurrent Neural Networks [1pt]

Solution. Let $\sigma = \frac{1}{1+\exp(-z)}$, and $\mathbf{x}_t = (x_1^t, x_2^t)$ denotes the input feature at time t. Note that when weights are sufficient large in scale, σ behaves like hard threshold function. Consider the following recurrent network:

$$\begin{aligned}
\hat{y}_t &= \sigma(\mathbf{w}_{hy}\mathbf{h}_t+b_y) && (4.1)\\
\mathbf{h}_t &= \sigma\left(\mathbf{w}_{xh}\mathbf{x}_t+\mathbf{w}_{hh}\mathbf{h}_{t-1}+\mathbf{b}_h\right) && (4.2)
\end{aligned}$$

with the following parameters:

$$\mathbf{w}_{xh} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \mathbf{w}_{hh} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \mathbf{b}_h = \begin{pmatrix} -0.5 \\ -1.5 \\ -2.5 \end{pmatrix} \tag{4.3}$$

$$\mathbf{w}_{hy} = \begin{pmatrix} 1 & 0 & 1 \end{pmatrix} \quad b_y = -0.5 \tag{4.4}$$

$$\mathbf{h}_t = \begin{pmatrix} \mathbb{1}\{x_1^t + x_2^t + h_{t-1} \geq 1\} \\ \mathbb{1}\{x_1^t + x_2^t + h_{t-1} \geq 2\} \\ \mathbb{1}\{x_1^t + x_2^t + h_{t-1} \geq 3\} \end{pmatrix} \tag{4.5}$$

Justification:

$$\mathbf{w}_{xh}\mathbf{x}_t = \begin{pmatrix} x_1^t + x_2^t \\ x_1^t + x_2^t \\ x_1^t + x_2^t \end{pmatrix} \quad \mathbf{w}_{hh}\mathbf{h}_{t-1} = \begin{pmatrix} \mathbb{1}\{x_1^{t-1} + x_2^{t-1} + h_{t-2} \geq 2\} \\ \mathbb{1}\{x_1^{t-1} + x_2^{t-1} + h_{t-2} \geq 2\} \\ \mathbb{1}\{x_1^{t-1} + x_2^{t-1} + h_{t-2} \geq 2\} \end{pmatrix} \tag{4.6}$$

Let c_t denote the carry from the previous significant figure. Therefore, elements in $\mathbf{w}_{hh}\mathbf{h}_{t-1}$ are one only if $c_t = 1$. Then,

$$\mathbf{h}_t = \sigma\left(\mathbf{w}_{xh}\mathbf{x}_t + \mathbf{w}_{hh}\mathbf{h}_{t-1} + \mathbf{b}_h\right) = \begin{pmatrix} \mathbb{1}\{x_1^t + x_2^t + c_t \geq 1\} \\ \mathbb{1}\{x_1^t + x_2^t + c_t \geq 2\} \\ \mathbb{1}\{x_1^t + x_2^t + c_t \geq 3\} \end{pmatrix} \tag{4.7}$$

For the output layer,

$$\hat{y}_t = \sigma\left(\mathbf{w}_{xh}\mathbf{x}_t + \mathbf{w}_{hh}\mathbf{h}_{t-1} + \mathbf{b}_h\right) = \mathbb{1}\{x_1^t + x_2^t + c_t \geq 1\} \vee \mathbb{1}\{x_1^t + x_2^t + c_t \geq 3\} \tag{4.8}$$

Therefore, let $c \in \{0, 1\}$ denote the carry, $\hat{y}$ whenever $x_1 + x_2 + c$ is one or three, and $\hat{y} = 0$ otherwise. ■