CSC413: Homework 3

Tianyu Du (1003801647)

2020/03/03 at 18:38:10

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:

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

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,

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

■

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

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

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

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

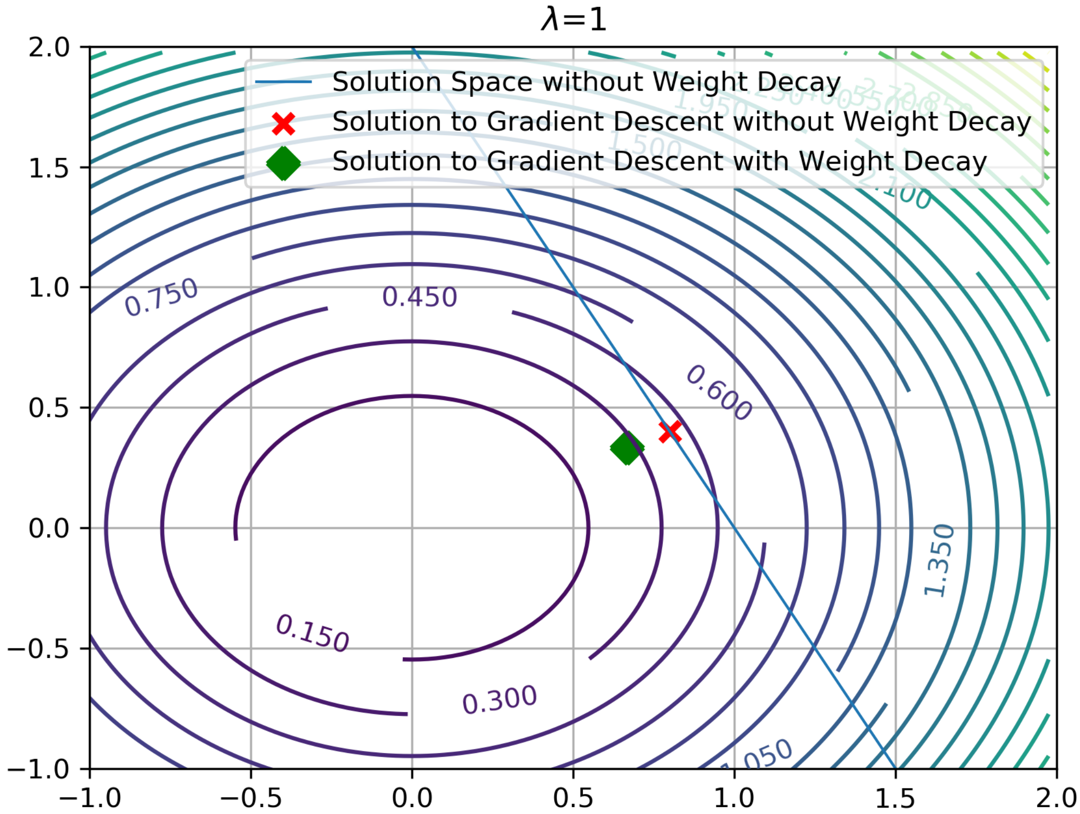
$$\implies \begin{cases} w_1^* & = \frac{4}{\lambda+5} \\ w_2^* & = \frac{2}{\lambda+5} \end{cases} \tag{1.16}$$

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]

Solution. ■

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. Suppose there are K different models indexed using $j \in \{1, 2, \cdots, K\}$:

$$h_j(\mathbf{x}) = \mathbf{w}_j(\mathcal{D}_j)\mathbf{x} \tag{2.1}$$

where $\mathcal{D}_j$ are i.i.d. realization of datasets. Let $\overline{h}(\mathbf{x})$ denote the weight average ensemble:

$$\begin{aligned} \overline{h}(\mathbf{x}) &= \overline{\mathbf{w}}\mathbf{x} & (2.2) \\ &= \sum_{j=1}^{K} \mathbf{w}_j(\mathcal{D}_j)\mathbf{x} & (2.3) \end{aligned}$$

And the prediction average at dataset point $\mathbf{x}$is simply

$$\sum_{j=1}^{K} h_j(\mathbf{x}) \tag{2.4}$$

Therefore, the prediction from weight-average and prediction-average ensembles are the same. Hence, the expected generalization error should be the same. ■

2.1.2 [0pt]

Solution. ■

2.2 Bagging - Uncorrelated Models

2.2.1 Bias with bagging [0pt]

Solution. Note that

$$\begin{aligned} \mathbb{E}\left[\bar{h}(\mathbf{x};\mathcal{D})|\mathbf{x}\right] &= \mathbb{E}\left[\frac{1}{k}\sum_{i=1}^{k} h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] & (2.5) \\ &= \frac{1}{k}\sum_{i=1}^{k} \mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] & (2.6) \end{aligned}$$

Since $\mathcal{D}_i$ are drawn from the identical distribution, so that

$$\mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] = \mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_j\right)|\mathbf{x}\right] \quad \forall i,j \in \{1,2,\cdots,k\} \tag{2.7}$$

Hence,

$$\mathbb{E}\left[\bar{h}(\mathbf{x};\mathcal{D})|\mathbf{x}\right] = \frac{1}{k}\sum_{i=1}^{k} \mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] = \mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] \quad \forall i \in \{1,2,\cdots,k\} \tag{2.8}$$

Since each data point in $\mathcal{D}_i$ is uniformly sampled with replaced from $\mathcal{D} \sim p_{\text{data}}$, therefore, $\mathcal{D}_i \sim p_{\text{data}}$ as well.

$$\mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}\right)|\mathbf{x}\right] = \mathbb{E}\left[h\left(\mathbf{x};\mathcal{D}_i\right)|\mathbf{x}\right] \quad \forall i \in \{1, 2, \cdots, k\} \tag{2.9}$$

Therefore,

$$bias = \mathbb{E}\left[\left|\mathbb{E}\left[\bar{h}(\mathbf{x};\mathcal{D})|\mathbf{x}\right] - y_*(\mathbf{x})\right|^2\right] = \mathbb{E}\left[\left|\mathbb{E}\left[h(\mathbf{x};\mathcal{D})|\mathbf{x}\right] - y_*(\mathbf{x})\right|^2\right] \tag{2.10}$$

■

2.2.2 Variance with bagging [1pt]

Solution. Suppose

$$\mathbb{E}\left[\left|h(\mathbf{x};\mathcal{D}) - \mathbb{E}\left[h(x;\mathcal{D})|\mathbf{x}\right]\right|^2\right] = \sigma^2 \tag{2.11}$$

For the bagging model,

$$\begin{aligned}
Var(\overline{h}) &= \mathbb{E}\left[\left|\overline{h}(\mathbf{x};\mathcal{D}) - \mathbb{E}\left[\overline{h}(x;\mathcal{D})|\mathbf{x}\right]\right|^2\right] && (2.12)\\
&= \mathbb{E}\left[\left|\frac{1}{k}\sum_{i=1}^{k} h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[\overline{h}(x;\mathcal{D})|\mathbf{x}\right]\right|^2\right] && (2.13)\\
&= \mathbb{E}\left[\left(\frac{1}{k}\sum_{i=1}^{k} h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[\overline{h}(x;\mathcal{D})|\mathbf{x}\right]\right)^2\right] && (2.14)
\end{aligned}$$

Since $\mathbb{E}\left[\overline{h}(x;\mathcal{D})|\mathbf{x}\right]$ is constant for all realizations of datasets $\mathcal{D}_i$ and equals $\mathbb{E}\left[h(x;\mathcal{D})|\mathbf{x}\right]$ by linearity of expectation.

$$\begin{aligned}
&= \mathbb{E}\left[\left(\frac{1}{k}\sum_{i=1}^{k}\left\{h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[h(x;\mathcal{D}_i)|\mathbf{x}\right]\right\}\right)^2\right] && (2.15)\\
&= \frac{1}{k^2}\mathbb{E}\left[\left(\sum_{i=1}^{k}\left\{h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[h(x;\mathcal{D}_i)|\mathbf{x}\right]\right\}\right)^2\right] \quad (\dagger) && (2.16)
\end{aligned}$$

Because datasets $\mathcal{D}_i$ are drawn independently,

$$\mathbb{E}\left[\left(h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[h(x;\mathcal{D}_i)|\mathbf{x}\right]\right)\left(h\left(\mathbf{x};\mathcal{D}_j\right) - \mathbb{E}\left[h(x;\mathcal{D}_j)|\mathbf{x}\right]\right)\right] = Cov(h_i, h_j) = 0 \tag{2.17}$$

Hence, after expanding the squared sum in (†),

$$\begin{aligned}
(\dagger) &= \frac{1}{k^2}\mathbb{E}\left[\sum_{i=1}^{k}\left(h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[h(x;\mathcal{D}_i)|\mathbf{x}\right]\right)^2\right] && (2.18)\\
&= \frac{1}{k^2}\sum_{i=1}^{k}\mathbb{E}\left[\left(h\left(\mathbf{x};\mathcal{D}_i\right) - \mathbb{E}\left[h(x;\mathcal{D}_i)|\mathbf{x}\right]\right)^2\right] && (2.19)\\
&= \frac{1}{k^2}\sum_{i=1}^{k} Var(h_i) && (2.20)
\end{aligned}$$

Since $\mathcal{D}_i$ are i.i.d. from the dataset, $Var(h_i) = Var(h)$ for every i, therefore,

$$Var(\overline{h}) = \frac{\sigma^2}{k} \tag{2.21}$$

■

2.3 Bagging - General Case

2.3.1 Bias under Correlation [1pt]

2.3.2 Variance under Correlation [0pt]

2.3.3 Intuitions on Bagging [1pt]

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

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

$$\implies w_2 = \frac{2\sigma^2}{2\sigma^2+1} \tag{3.14}$$

$\blacksquare$

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

Solution. Let G_1, G_2, G_3 denote the three Gaussian distributions respectively, so that

$$X_1 \leftarrow G_1 \tag{3.15}$$
$$Y \leftarrow X_1 + G_2 \tag{3.16}$$
$$X_2 \leftarrow Y + G_3 \tag{3.17}$$

So that,

$$\begin{aligned}\mathcal{J} &= \mathbb{E}_{(x_1,x_2,y)\sim(X_1,X_2,Y)}[(y-\hat{y})^2] && (3.18)\\ &= \mathbb{E}[G_1 + G_2 - w_1 G1 - w_2(G_1 + G_2 + G_3)]^2 && (3.19)\\ &= \mathbb{E}[(1 - w_1 - w_2)G_1 + (1 - w_2)G_2 - w_2 G_3]^2 && (3.20)\\ &= (1 - w_1 - w_2)^2\sigma^2 + (1 - w_2)^2\sigma^2 + w_2^2 && (3.21)\end{aligned}$$

For w_1:

$$\frac{\partial}{\partial w_1}\mathcal{J} = -2(1 - w_1 - w_2)\sigma^2 = 0 \tag{3.22}$$

For w_2:

$$\frac{\partial}{\partial w_2}\mathcal{J} = -2(1 - w_1 - w_2)\sigma^2 - 2(1 - w_2)\sigma^2 + 2w_2 = 0 \tag{3.23}$$

Solving two equations:

$$w_1 = \frac{1}{\sigma^2 + 1} \tag{3.24}$$
$$w_2 = \frac{\sigma^2}{\sigma^2 + 1} \tag{3.25}$$

$\blacksquare$

3.1.4 Different σs [0pt]

Solution. $\blacksquare$

3.2 Dropout as Data-Dependent $L2$ Regularization

3.2.1 Expectation and variance of predictions [0pt]

Solution. Let

$$\tilde{y} = 2\left(m_1 w_1 x_1 + m_2 w_2 x_2\right) \tag{3.26}$$

Then

$$\mathbb{E}\left[\tilde{y}\right] = \mathbb{E}\left[2\left(m_1 w_1 x_1 + m_2 w_2 x_2\right)\right] \tag{3.27}$$

■

3.3 Effect on Dropout [1pt]

Solution. Using bias-variance decomposition of the generalization error:

$$\begin{aligned}
\mathbb{E}[\tilde{\mathcal{L}}] &= \mathbb{E}[(\tilde{y}-y)^2] && (3.28)\\
&= \mathbb{E}\left[(\mathbb{E}_m[\tilde{y}]-y)^2\right] + Var(\hat{y}) && (3.29)\\
&= \mathbb{E}\left[(\hat{y}-y)^2\right] + Var(2\,(m_1w_1x_1+m_2w_2x_2)) && (3.30)\\
&= \mathbb{E}\left[(\hat{y}-y)^2\right] + 4Var\left[m_1w_1x_1+m_2w_2(x_1+G_2+G_3)\right] && (3.31)\\
&= \mathbb{E}\left[(\hat{y}-y)^2\right] + 4Var\left[(m_1w_1+m_2w_2)x_1+m_2w_2(G_2+G_3)\right] && (3.32)
\end{aligned}$$

Therefore, adding the dropout is equivalent to adding a regularization term in which the level of plenty (λ_j) for each w_j depends on the variance of x_j. And such regularization would help the model achieve a better generalization error. ■

Should look like a regularization, but check how to derive it.

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:

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

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

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

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. ■