Training and Generalization

- Overfitting, Underfitting, and Goldilocks Fitting
- Training, Validation, and Testing Data Sets
- Model Order, Model Capacity, Generalization Loss

Training and Generalization

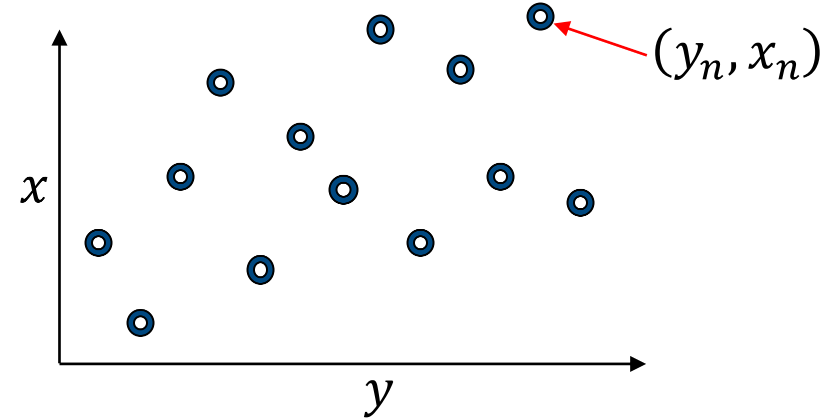
- Goal:
  - Learn the "true relationship" from training data pairs $(x_k, y_k)|_{k=0}^{K-1}$.

$$x = f_\theta(y) + error$$

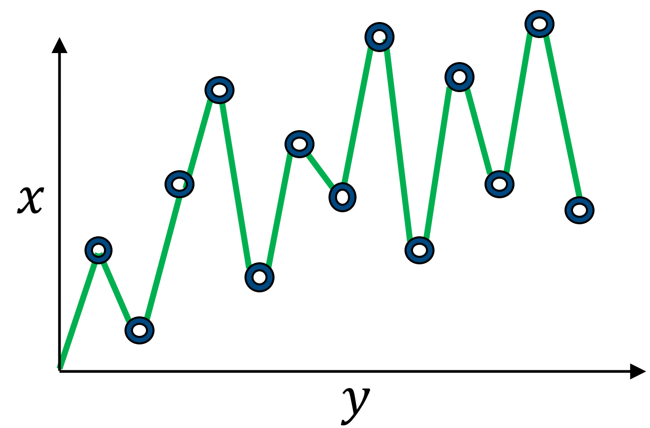
  - What we learn needs to *generalize* beyond the training data.
- Key parameters:
  - P = <u>Model Order</u> = number of parameters = Dimension of $\theta \in \Re^P$
  - $N_x \times K$ = # training points = (Dimension of x) × (# of training pairs)
- Key issues
  - If $P \gg N_x \times K$: Model order is too high and there is a tendency to over fit.
  - If $P \ll N_x \times K$: Model order is too low, and there is a tendency to under fit.

Overfitting

- Training data



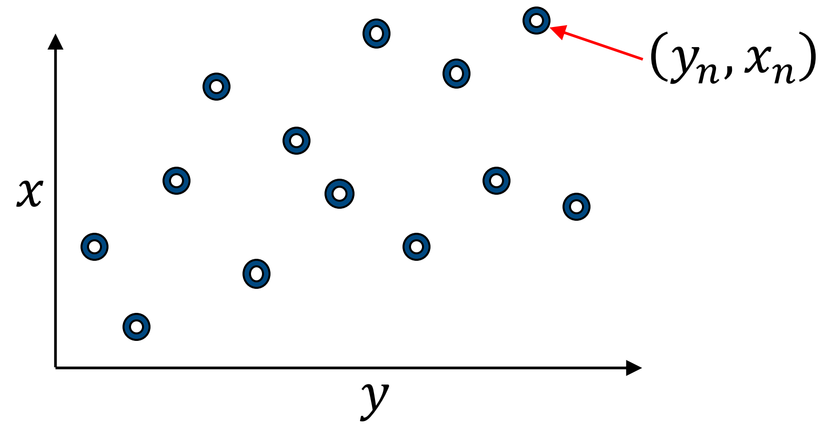
- Overfitting



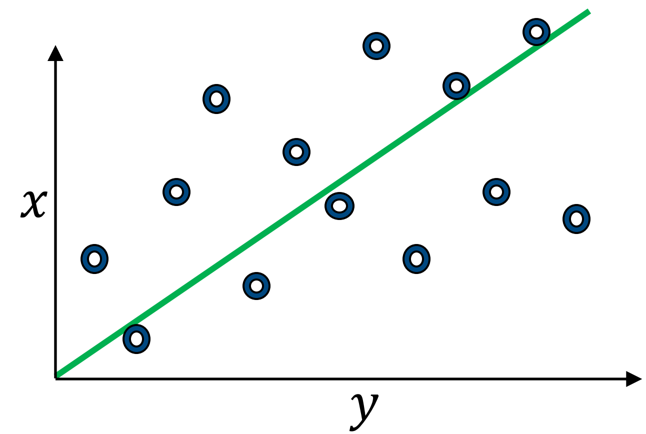
  – Model order too high
  – Doesn't generalize well

Underfitting

- Training data



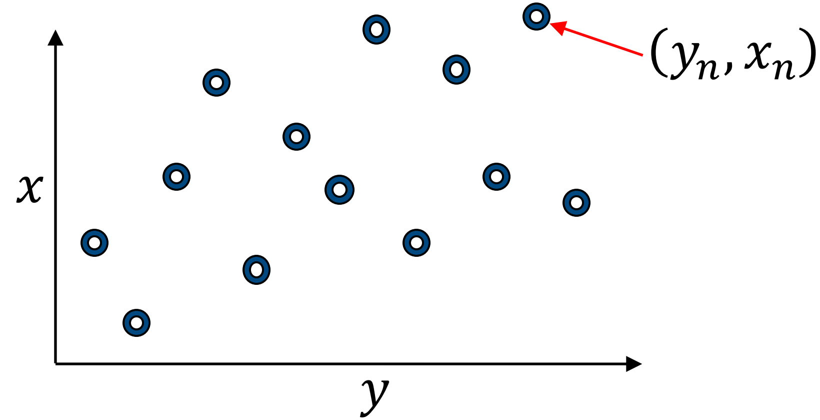
- Underfitting



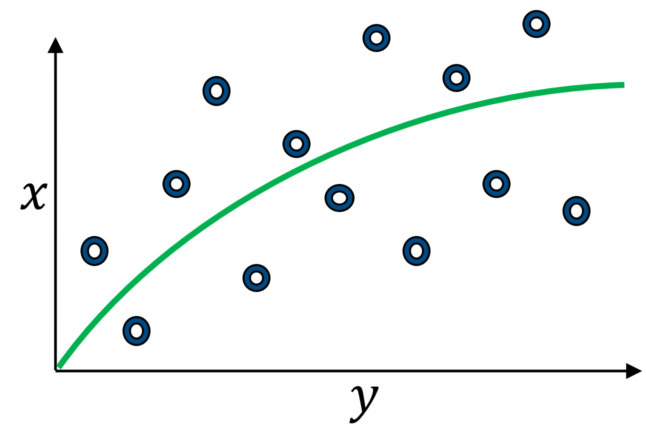
  – Model order too low
  – Doesn’t generalize well

Goldilocks Fitting

- Training data



- Best fitting



  - Model order “just right”
  - Best generalization

Partitioning of Labeled Data

- Let (x_k, y_k) for k $\in S = \{0, \cdots, K-1\}$ be the full set data.
  - y_k is the input data.
  - x_k is the label or "ground truth" data.
- Typically, we <u>randomly</u> partition* the data into three subsets:
  - S_T is the <u>training</u> data
  - S_V is the <u>validation</u> data
  - S_E is the <u>testing</u> (<u>evaluation</u>) data

    * Note that "partition" means $S = S_\mathrm{T} \cup S_V \cup S_E$ and $\emptyset = S_T \cap S_V = S_T \cap S_E = S_V \cap S_E$
- For each partition, we define a loss function:

$$L_T(\theta) = \frac{1}{|S_T|} \sum_{k \in S_T} \|x_k - f_\theta(y_k)\|^2$$

$$L_V(\theta) = \frac{1}{|S_V|} \sum_{k \in S_V} \|x_k - f_\theta(y_k)\|^2$$

$$L_E(\theta) = \frac{1}{|S_E|} \sum_{k \in S_E} \|x_k - f_\theta(y_k)\|^2$$

Roles of Data

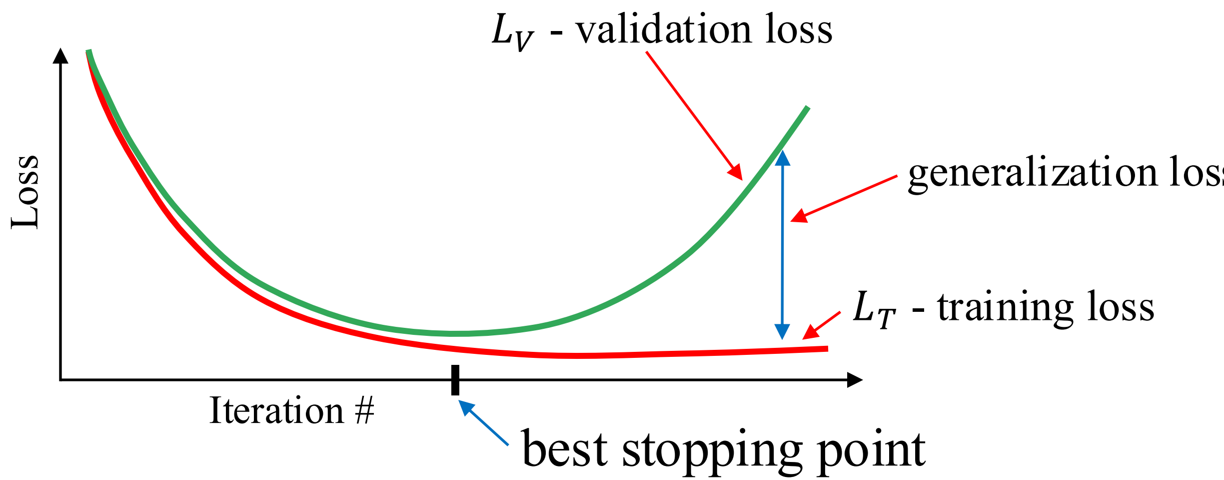
- Training data:
  - Only data used to train model

$$\theta^* = \arg\min_{\theta}\{L_T(\theta)\}$$
$$= \arg\min_{\theta}\left\{\frac{1}{K}\sum_{k\in S_T}\|x_k - f_\theta(y_k)\|^2\right\}$$

- Validation data:
  - Used to compare models of different order.
- Testing data
  - Used for final evaluation of model performance.

Loss Function Convergence

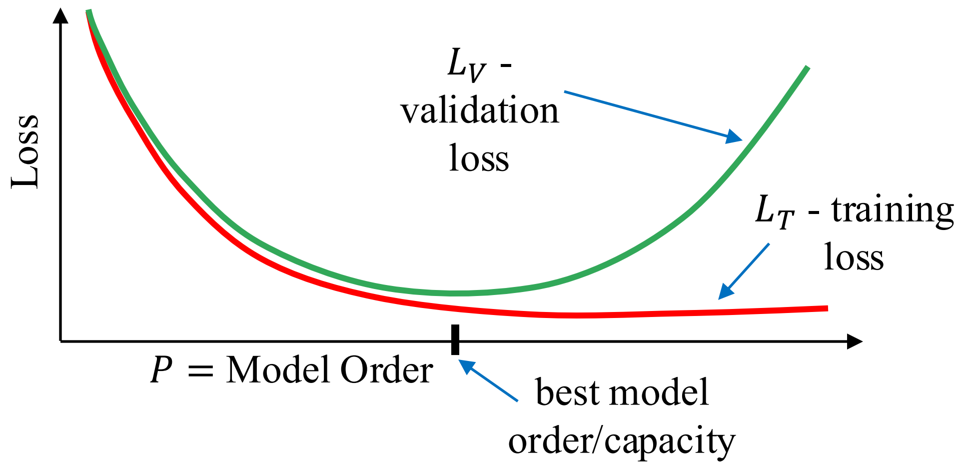
- Loss vs. iterations of gradient-based optimization



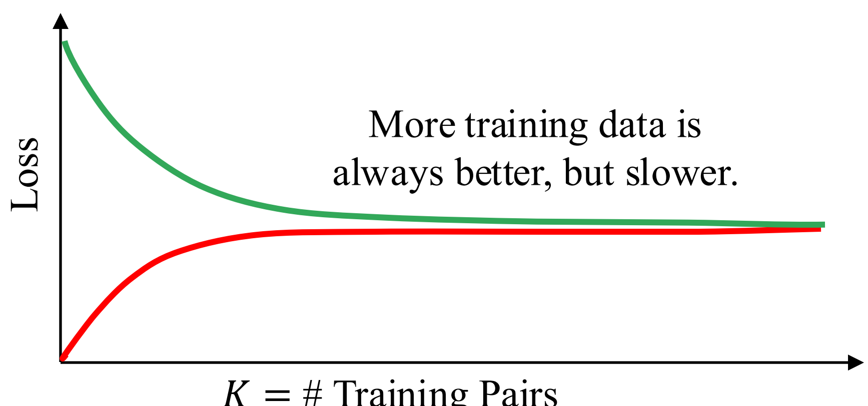
- Notice:
  - As training continues, the model is <u>overfit</u> to the data
  - Best to stop training when L_V is at a minimum
  - Model order is too high, but early termination of training can help fix problem

Loss vs. Model Order vs. # Training Pairs

- Loss vs. model order

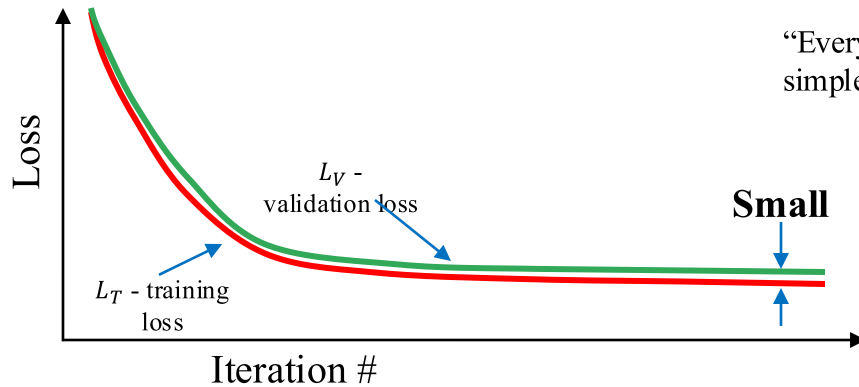


- Loss vs. # of training pairs



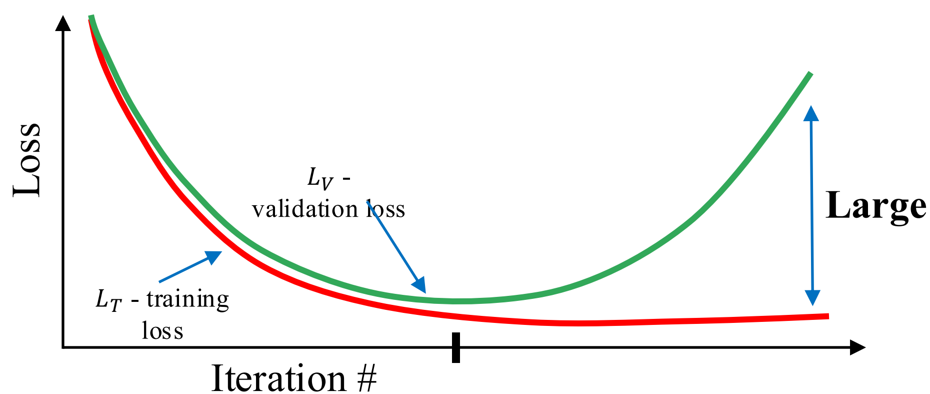
What are L_T and L_V telling you?

- Model order/model <u>capacity</u> may be too low…



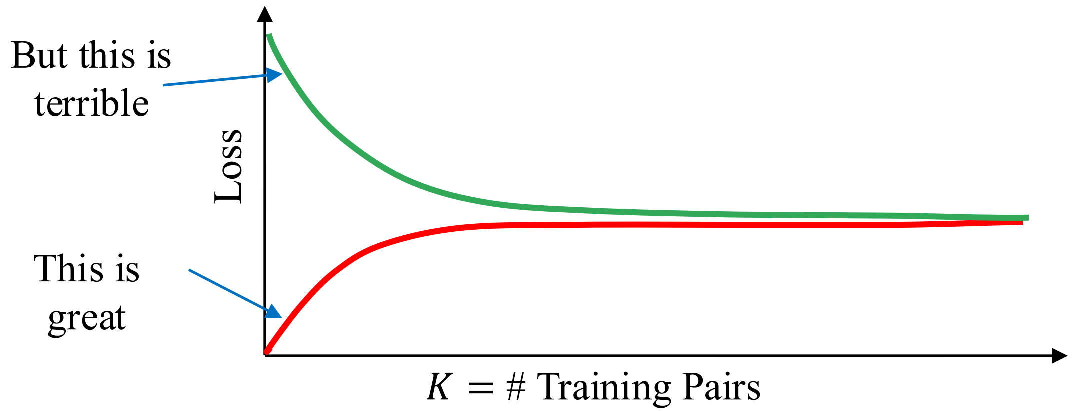
"Everything should be made as simple as possible, but no simpler,"
-Inspired by Albert Einstein

- Model order/model <u>capacity</u> may be too high…



Never Test on Training Data!

- Never report training loss, L_T, as your ML system accuracy!



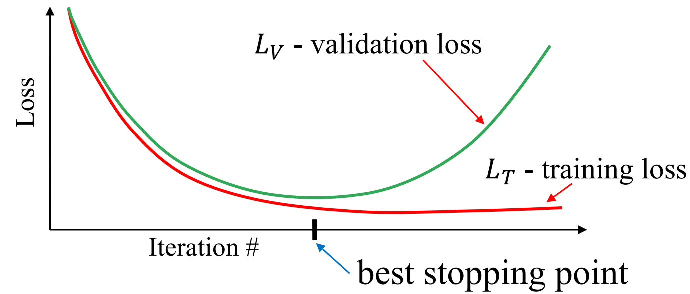
  - This is like doing a homework problem after you have seen the solution.
  - The network has "memorized" the answers.

- Don't ever report validation loss, L_V, as your ML system accuracy.
  - This is also biased by the fact that your tuned model order parameters.

- Only report <u>testing loss</u>, L_E, as your ML system accuracy.
  - This data is sequestered to ensure it is an unbiased estimate of loss.

Solutions to Parameter Overfitting

1. Early termination



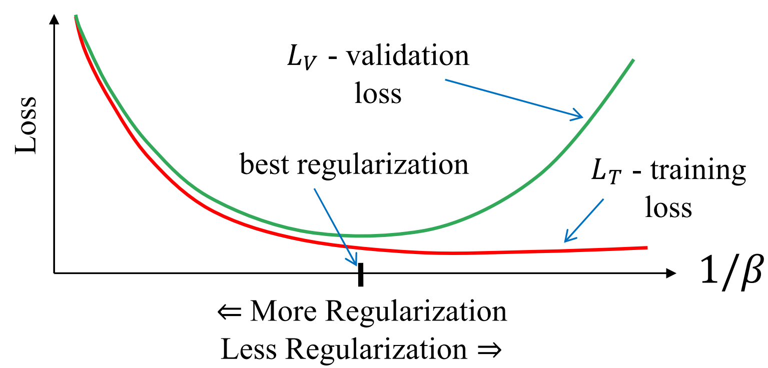
2. Regularization
   - L_2 and L_1 weight regularization
   - Loss function is modified to be

$$\tilde{L}(\theta) = L(\theta) + \beta\, S(\theta)$$

   - β larger $\Rightarrow$ less overfitting

L_2 norm - $S(\theta) = \|\theta\|^2$

L_1 norm - $S(\theta) = \|\theta\|_1$



3. Dropout Method: Next slide

Regularization and Dropout

- Weight Regularization and Initialization
- Dropout Methods

Regularized Maximum Likelihood

- Regularize ML estimate:

$$\hat{\theta} = \arg\min_{\theta}\{-\log p_\theta(x,y) + \beta\, S(\theta)\}$$

where $S(\theta)$ is a "regularizing" function, and β is the regularization weight.

Typical choices are

$$S(\theta) = -\log p(\theta)$$

MAP estimate

$$S(\theta) = \|\theta\|^2$$

Like a Gaussian Prior
Reduces amplitude of weights

$$S(\theta) = \|\theta\|_1$$

Like a Laplacian Prior
Encourages weights to go to zero

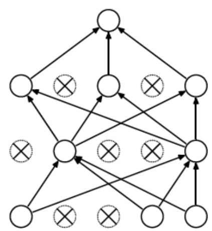
- Modified Loss function

$$\tilde{L}(\theta) = L(\theta) + \beta\, S(\theta)$$

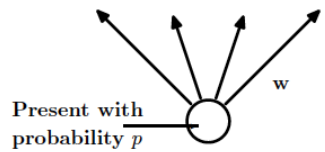
  - Can be interpreted as MAP estimate with $p(\theta) = \frac{1}{z}\exp\left\{-\frac{\beta}{2}S(\theta)\right\}$
  - Introduces bias into the estimate of θ
  - Reduces overfitting
  - Use regularization if training error >> validation error

The Dropout Method*

- Drop nodes with probability $1 - p \approx 0.2$
- Retain nodes with probability $p \approx 0.8$
- Scale all node outputs by p:
  - To compute loss for validation and test
  - During inference

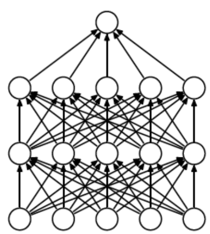


(b) After applying dropout.

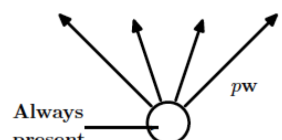


(a) At training time

During Training: Done independently for each batch



(a) Standard Neural Net



(b) At test time

During Validation, Testing, and Inference

*[Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, Ruslan Salakhutdinov, "Dropout: A Simple Way to Prevent Neural Networks from Overfitting", vol. 15, no. 56, pp. 1929−1958, 2014.]

Dropout: Training Algorithm

For each batch{
  For each layer l {
    $r^{(l)} \leftarrow Bernoulli(p, shape(y^{(l)}))$
  }
  For $n = 0$ to $K_b - 1$ {
    For each layer l {
      $\boxed{\tilde{y}^{(l)} \leftarrow r^{(l)} .* y^{(l)}}$
      $z^{(l+1)} \leftarrow w^{(l+1)} * \tilde{y}^{(l)}$
      $y^{(l+1)} \leftarrow f\left(z^{(l+1)}\right)$
    }
  }
}

Dropout

Training

- Dropouts are:
  - Independent for each internal node in the network
  - A single set of Bernoulli weights are computed for each batch.

Dropout: Validation and Testing

For each batch{
For $n = 0$ to $K_b - 1$ {
For each layer l {
$\boxed{\tilde{y}^{(l)} \leftarrow p * y^{(l)}}$
$z^{(l+1)} \leftarrow w^{(l+1)} * \tilde{y}^{(l)}$
$y^{(l+1)} \leftarrow f\left(z^{(l+1)}\right)$
}
}
}

scaling

Training

- Scale output to account for increased number of nodes

Dropout: Stochastic Generator

- Dropouts can be used to generate stochastic outputs for generators described later in class.
  - Leave dropouts on during inference
  - Output of DNN is then a random vector

$$\underbrace{\boxed{X}}_{\textit{Random Vector}} = f_\theta(\underbrace{\boxed{y}}_{\textit{Deterministic Input}})$$