OUTLINE

1. ~~Introduction~~
2. ~~Background~~
3. **Fitting a Model**
   - How to minimize a function?
   - Backpropagation
   - Improved Gradient Descent
   - The PyTorch Framework
4. Supervised Learning
5. Unsupervised Learning
6. Fantastic DNNs: How to choose them, how to train them

OUTLINE

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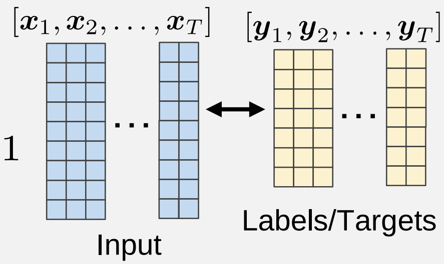
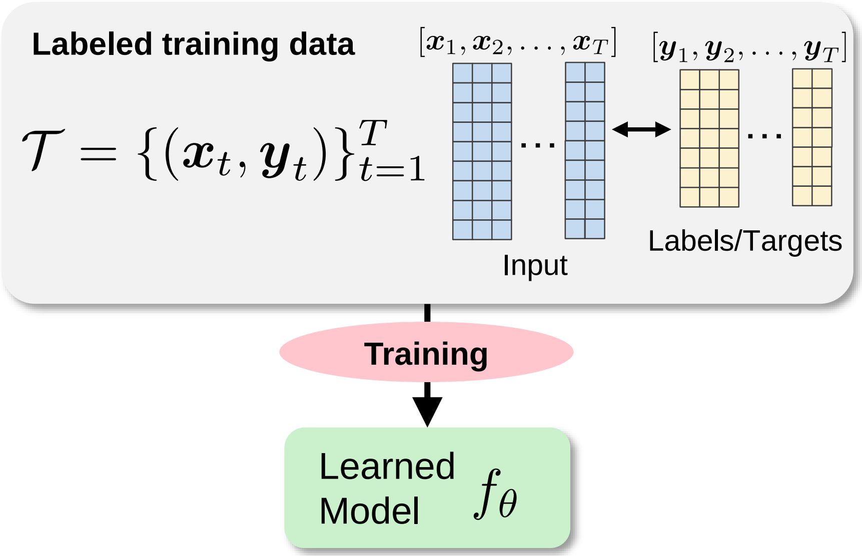
Supervised Learning

Labeled training data

$$\mathcal{T} = \{(\boldsymbol{x}_t, \boldsymbol{y}_t)\}_{t=1}^{T}$$



Supervised Learning



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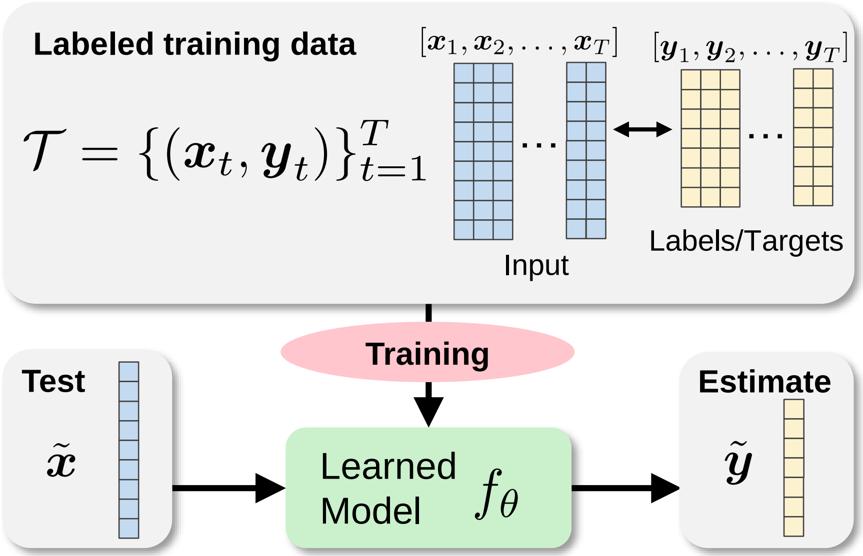

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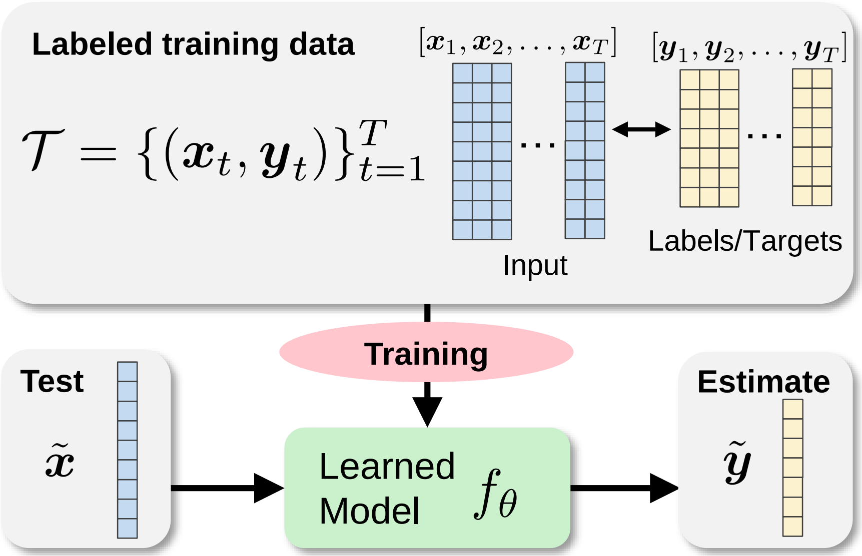


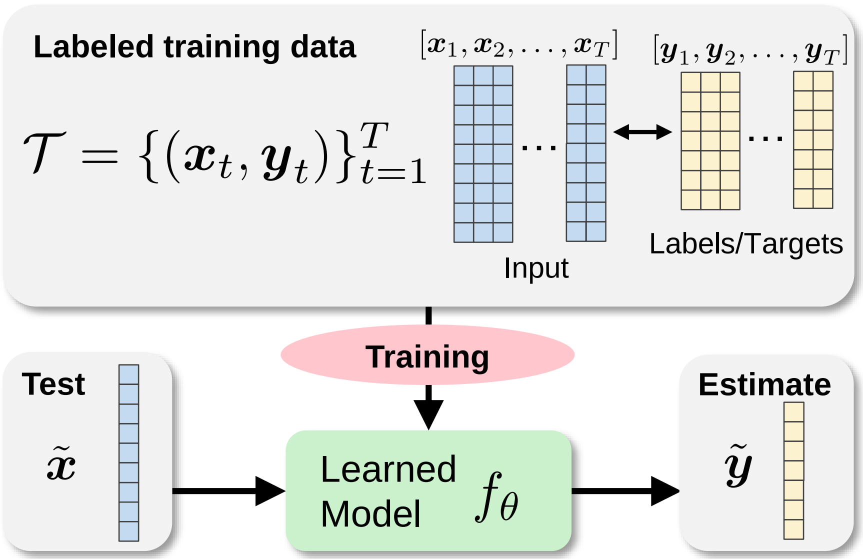
1. Discrete case: («one-hot»)
- Classification

Ex. application: *dog breed*

$\boldsymbol{y} =$

13: German Shepherd

Supervised Learning



1. Discrete case: («one-hot»)
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Ex. application: *dog breed*

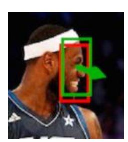
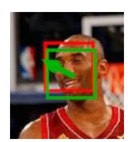
$\boldsymbol{y} =$ 1


13: German Shepherd

2. Continuous case:
- Regression

Ex. application: *head pose*

$\boldsymbol{y} =$

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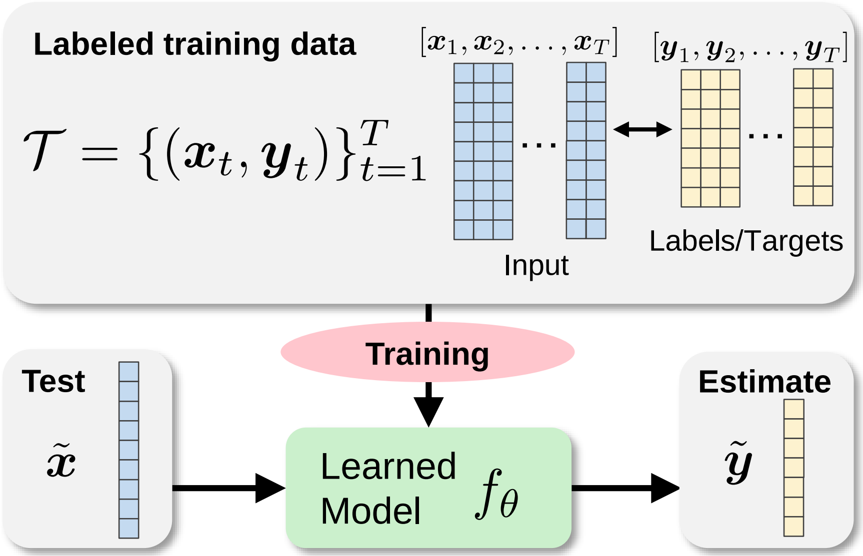

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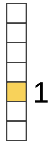
$\boldsymbol{y} =$ 

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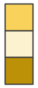
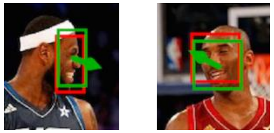
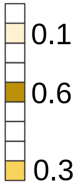
$\boldsymbol{y} =$ 

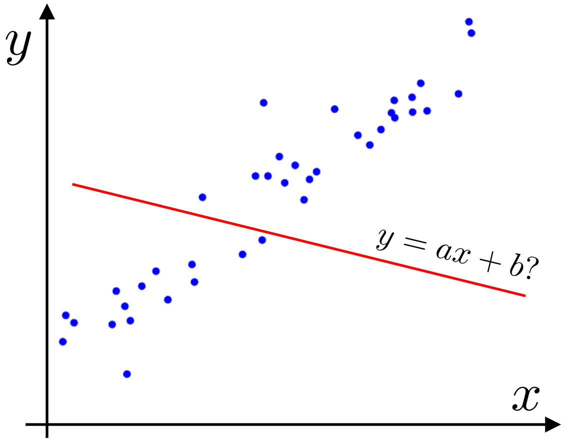


3. Sparse case:
- Multi-label classification

Ex. application: *image labelling*

$\boldsymbol{y} =$ 

Generalizing linear regression



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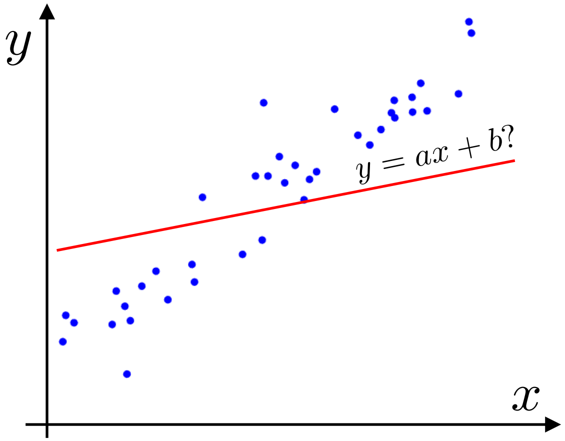

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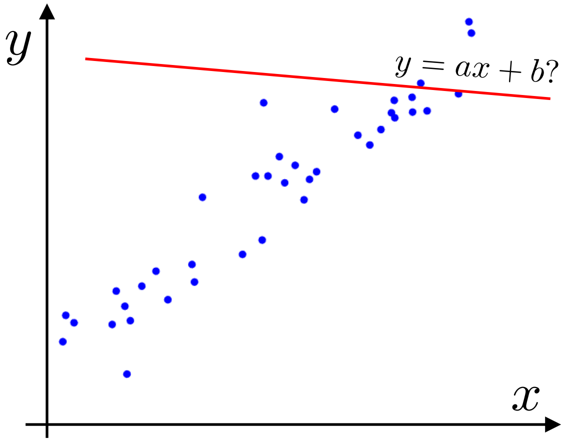

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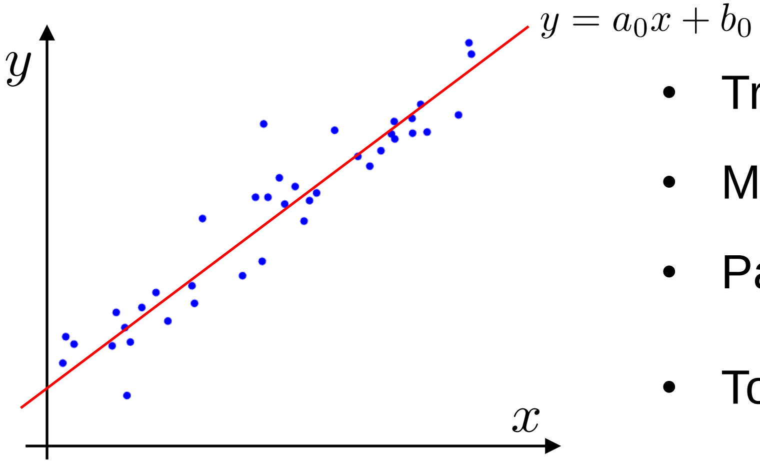

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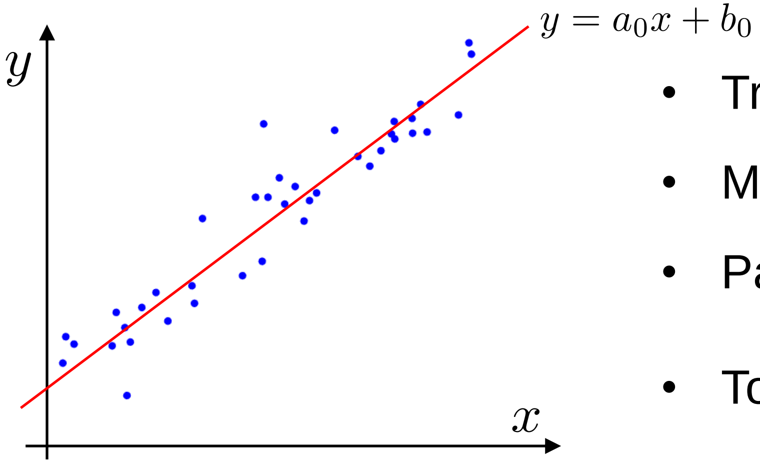

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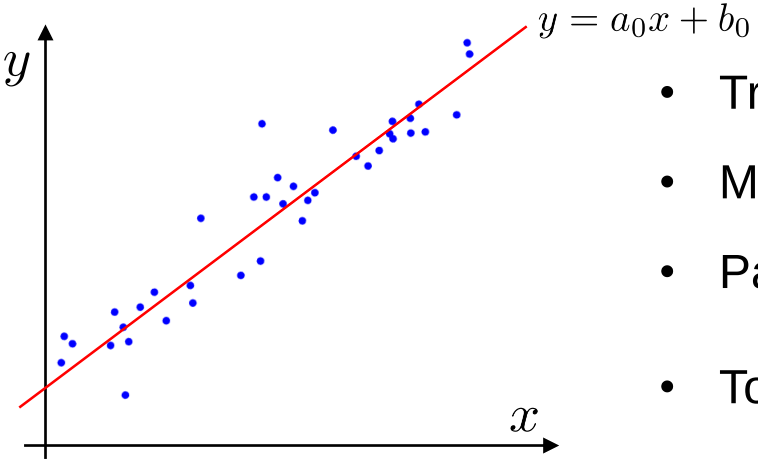
$$g(\boldsymbol{\theta}) = \frac{1}{T}\sum_{t=1}^{T}\Bigg(\underbrace{[x_t, 1]^\top}_{\boldsymbol{w}_t \in \mathbb{R}^2}\begin{bmatrix} a \\ b \end{bmatrix} - y_t\Bigg)^2 = \frac{1}{T}\|\mathbf{W}\boldsymbol{\theta} - \boldsymbol{y}\|_2^2, \quad \nabla_\theta g(\boldsymbol{\theta}_0) = \mathbf{0} \Rightarrow \boldsymbol{\theta}_0 = (\mathbf{W}^\top\mathbf{W})^{-1}\mathbf{W}^\top\boldsymbol{y}$$

Generalizing linear regression



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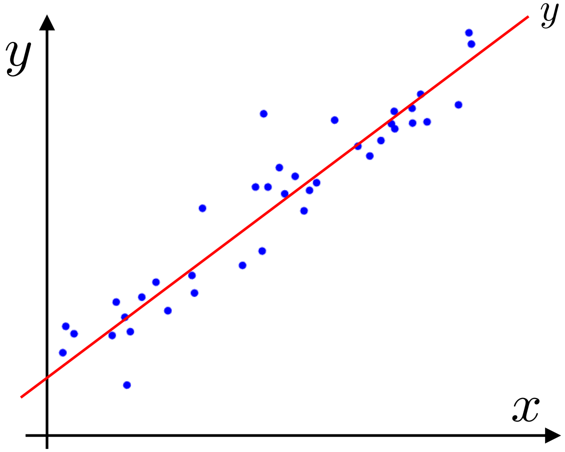
Generalizing linear regression



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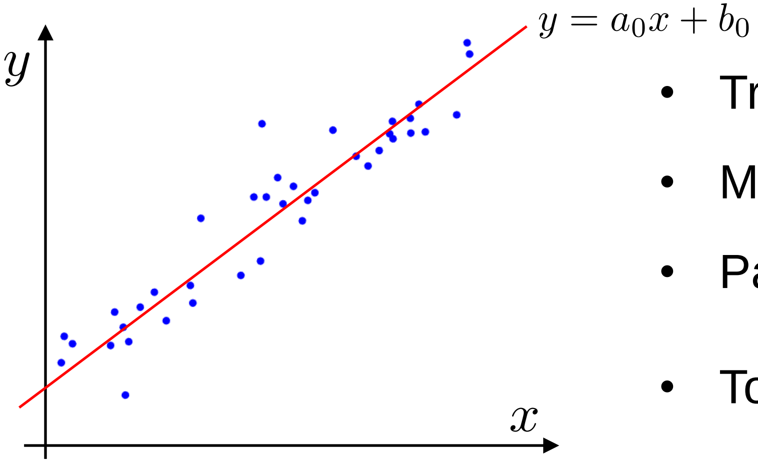
Generalizing linear regression



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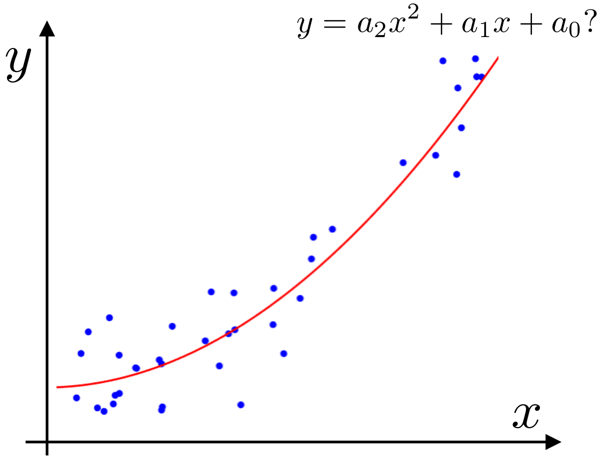
$$\mathbf{W} = \begin{bmatrix} \boldsymbol{x}_1^\top, & 1 \\ \vdots & \vdots \\ \boldsymbol{x}_T^\top, & 1 \end{bmatrix} \in \mathbb{R}^{T\times(D+1)}$$

Generalizing linear regression



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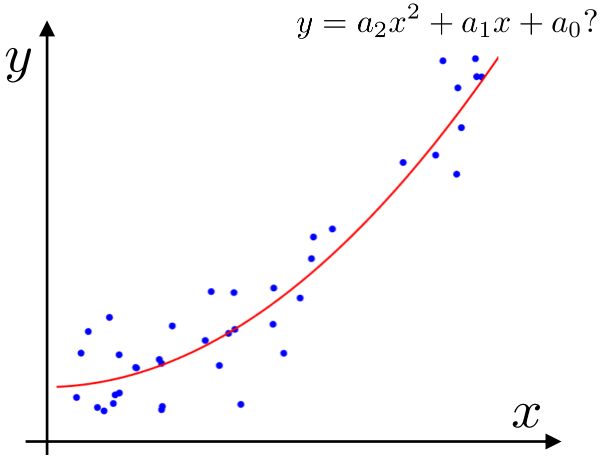
→ What about polynomial regression?

Generalizing linear regression



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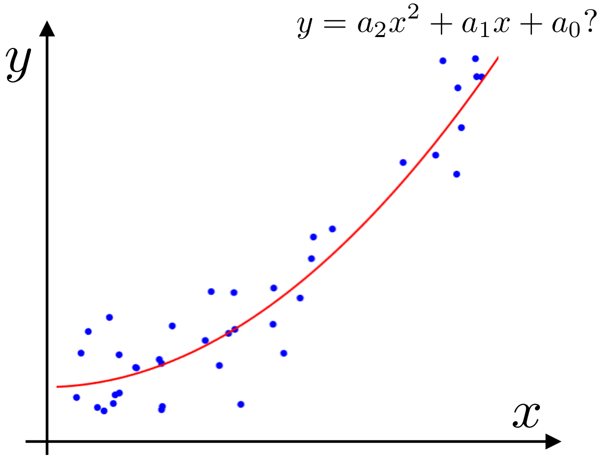
- Convertible to the **same problem** using the ***lifting***: $y = [a_0, a_1, a_2] \times \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}$

Generalizing linear regression



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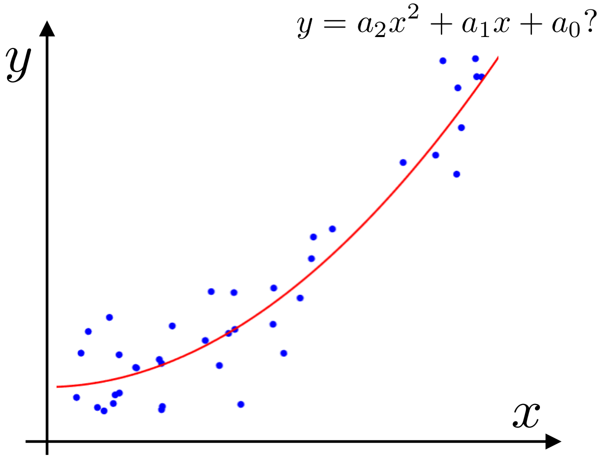
- More generally, 2^{nd} degree **multivariate** polynomial regression $(\boldsymbol{y} \in \mathbb{R}^N, \boldsymbol{x} \in \mathbb{R}^D)$:

$$y_n = \sum_{i=1}^{D}\sum_{j=i}^{D} a_{ij}^{(n)} x_i x_j + \sum_{i=1}^{D} a_i^{(n)} x_i + a_0^{(n)} \Rightarrow y_n = [a_0^{(n)}, a_1^{(n)}, \dots, a_{11}^{(n)}, a_{12}^{(n)} \dots, a_{DD}^{(n)}] \times \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_1^2 \\ x_1x_2 \\ \vdots \\ x_D^2 \end{bmatrix}$$

Generalizing linear regression



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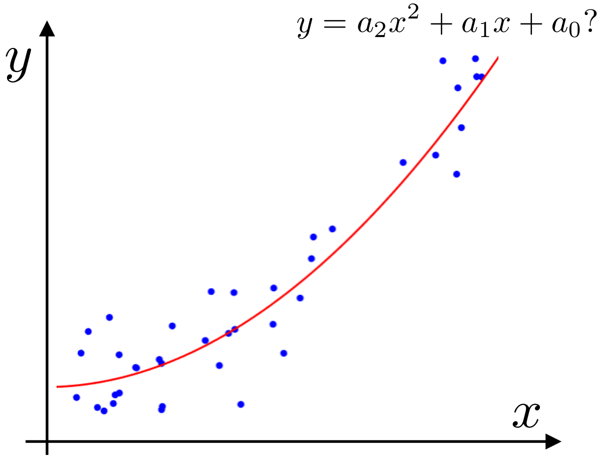
→How many parameters?

Generalizing linear regression



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→*How many parameters?* $\mathcal{O}(ND^2)$

Generalizing linear regression

- K[th] degree multivariate polynomial regression:

$$y_n = \sum_{i_1=1}^{D} \sum_{i_2=i_1}^{D} \cdots \sum_{i_K=i_{K-1}}^{D} a^{(n)}_{i_1 i_2 \dots i_K} x_{i_1} x_{i_2} \dots x_{i_K} + \cdots + \sum_{i_1=1}^{D} \sum_{i_2=i_1}^{D} a^{(n)}_{i_1 i_2} x_{i_1} x_{i_2} + \sum_{i_1=1}^{D} a^{(n)}_{i_1} x_{i_1} + a^{(n)}_0$$

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Generalizing linear regression

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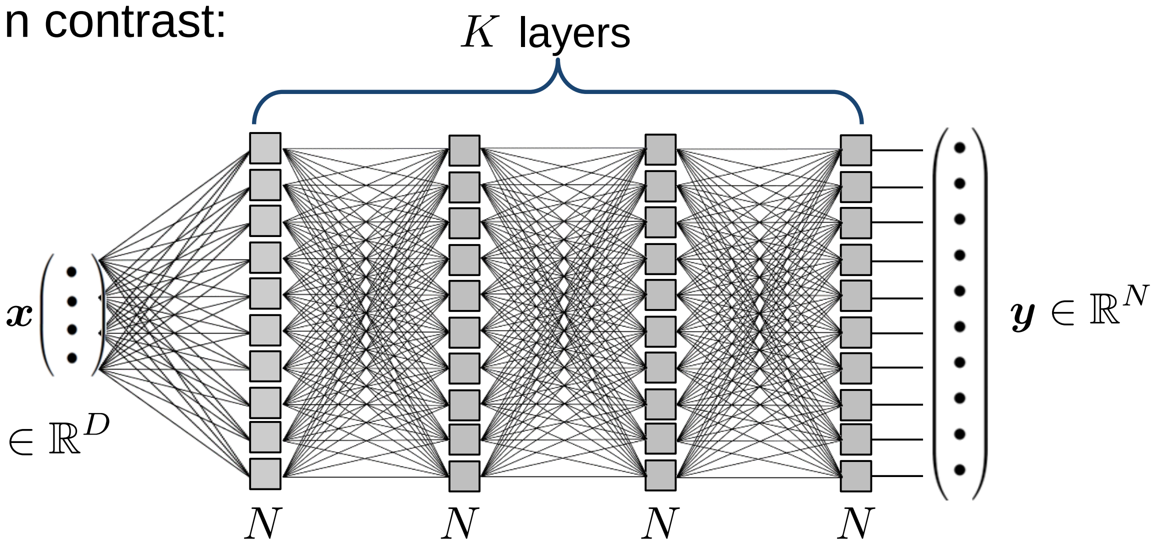
→How many parameters? $\mathcal{O}(ND^{K})$

- In contrast:



→How many parameters?

Generalizing linear regression

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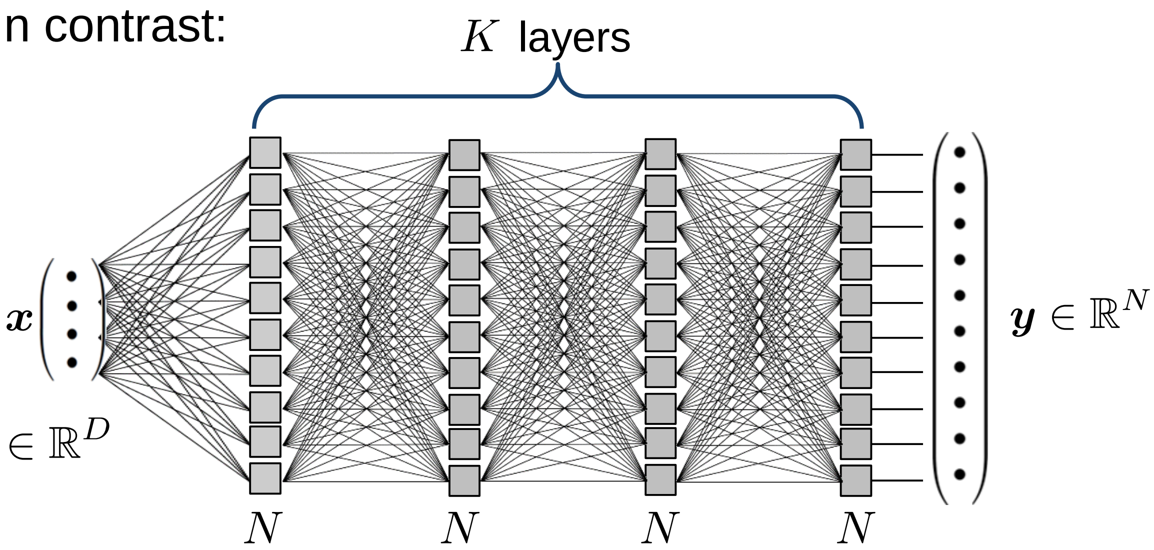
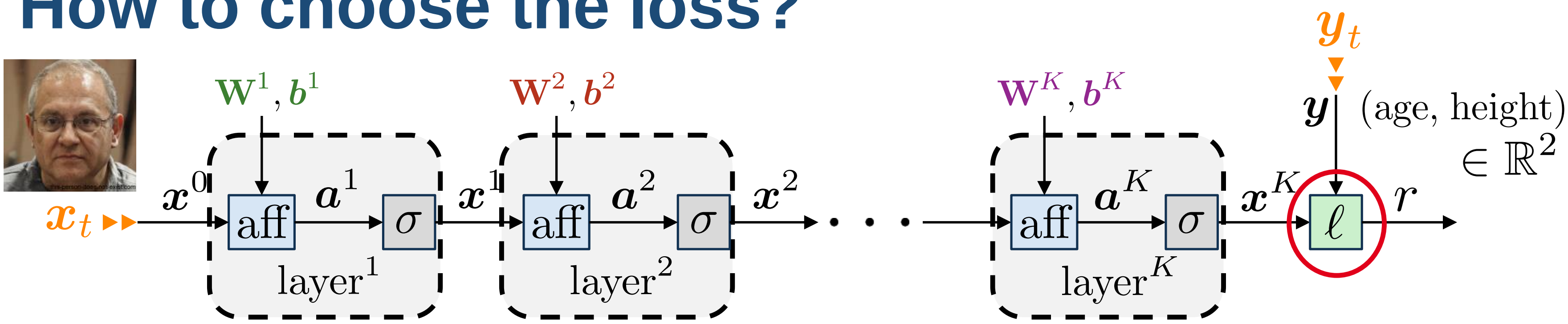


→How many parameters?

$$\mathcal{O}(DN + (K-1)N^2)$$

How to choose the loss?



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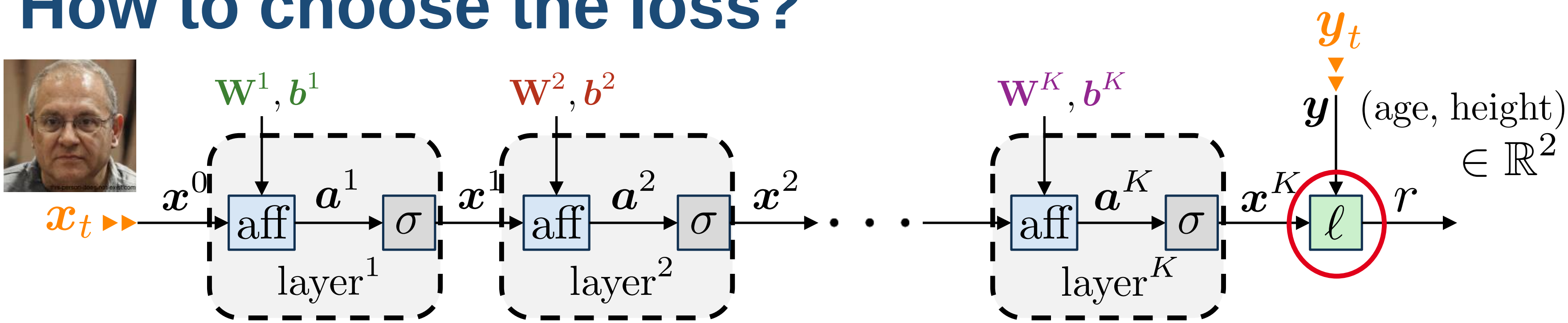
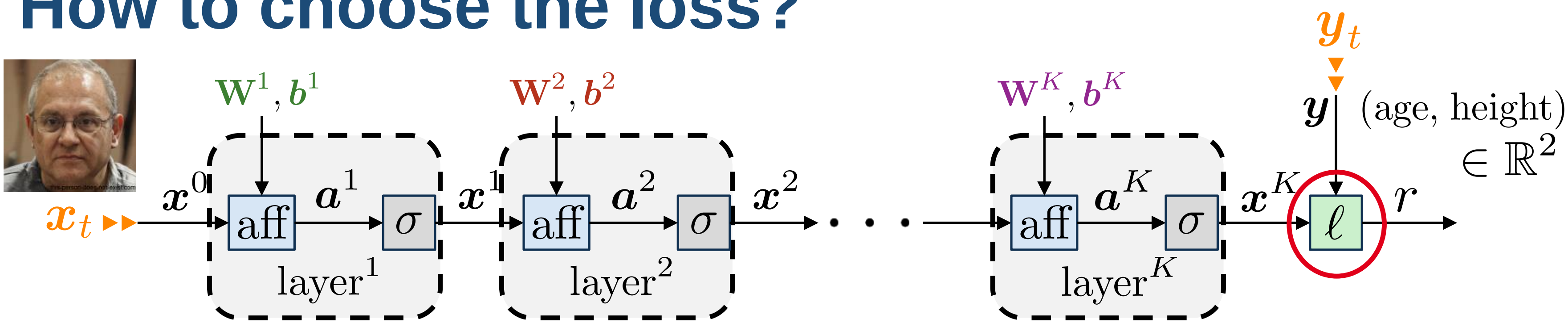


A general principled approach is to use the network to model $p(\boldsymbol{y}|\boldsymbol{x})$.

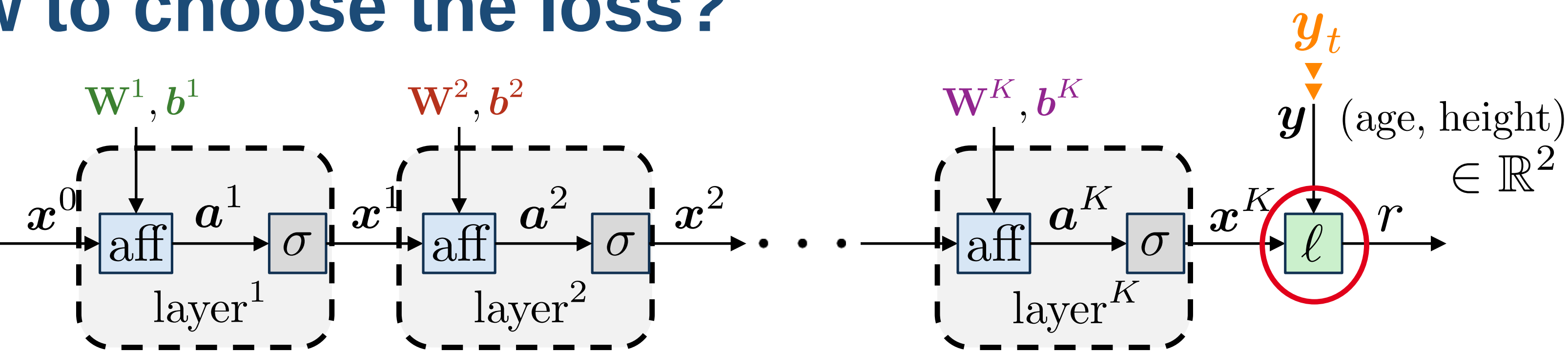
How to choose the loss?



A general principled approach is to use the network to model $p(\boldsymbol{y}|\boldsymbol{x})$.

1) Choose a **simple** family of **parameterized** probabilistic distributions over the domain of $\boldsymbol{y}$ and $\boldsymbol{x}^K$, i.e., $\mathcal{P} = \{\tilde{p}_\lambda(\boldsymbol{y})\}_{\lambda\in\Lambda}$.

How to choose the loss?



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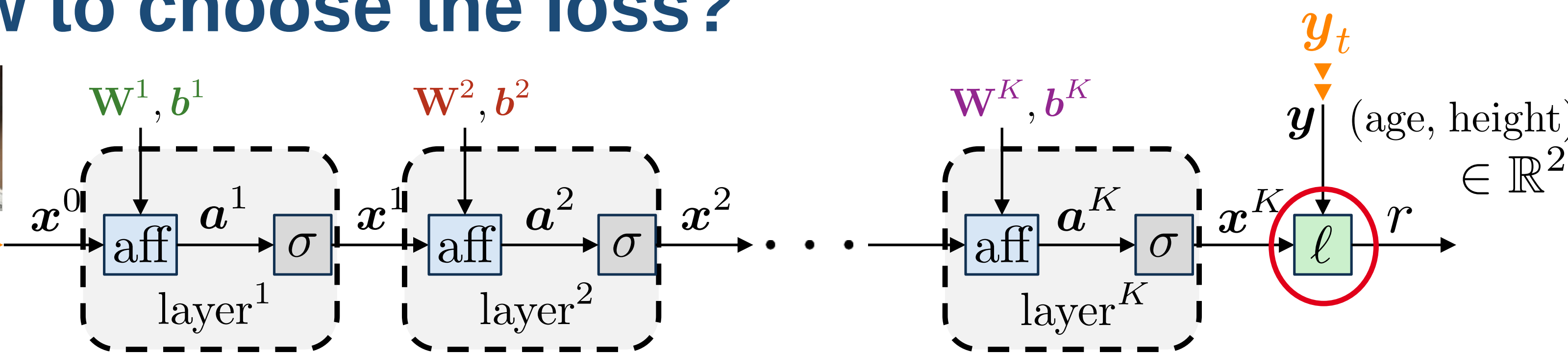

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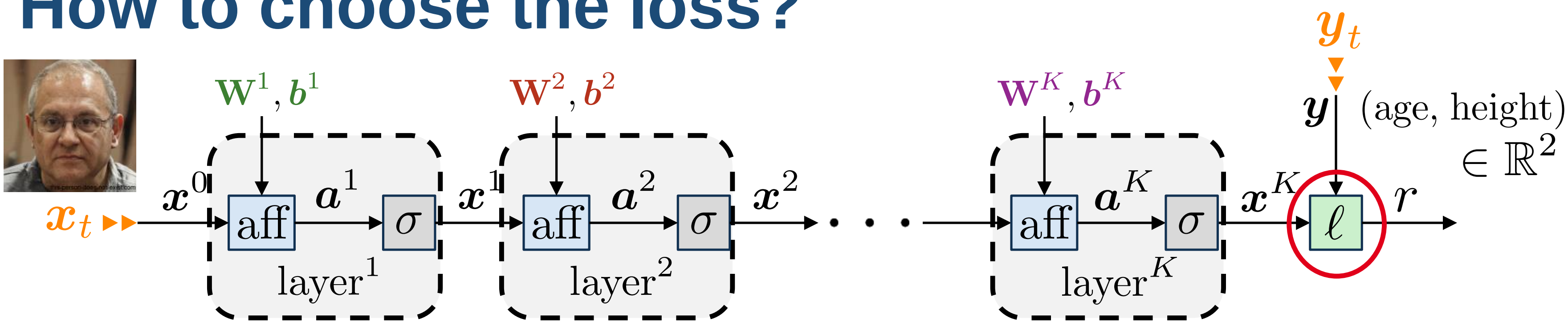

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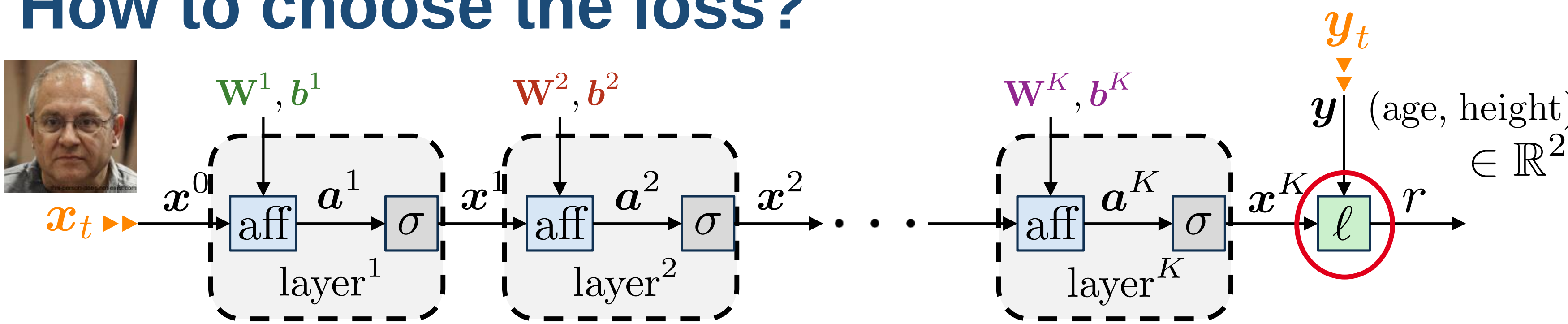

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Note: we assume the training set examples are **independent**.

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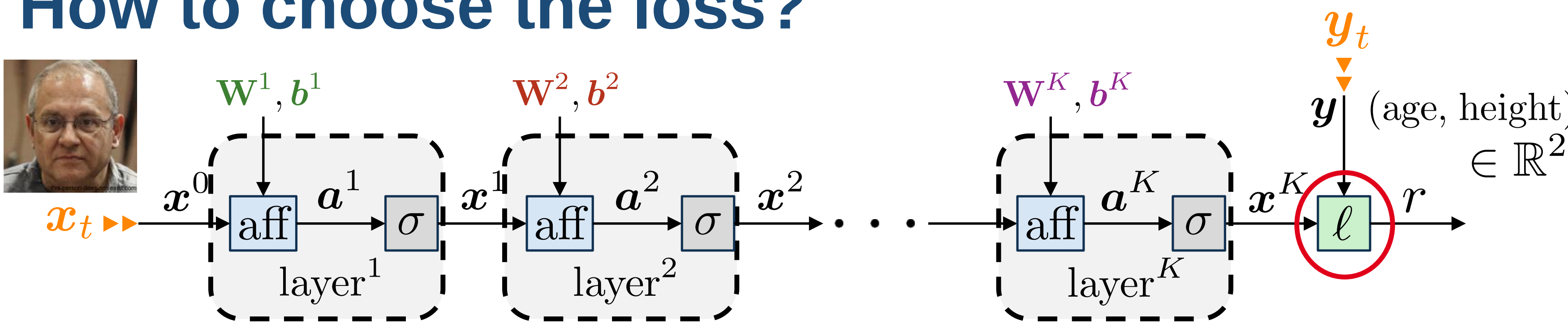

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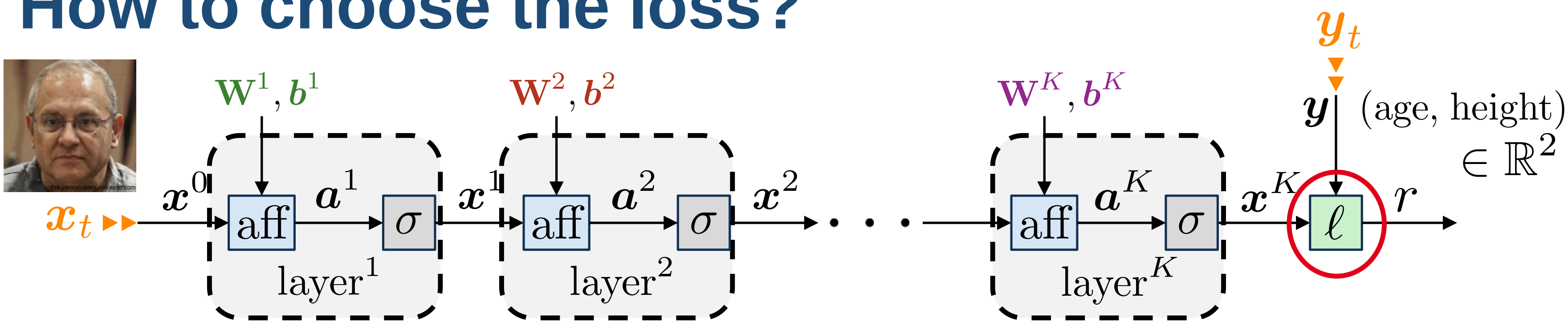

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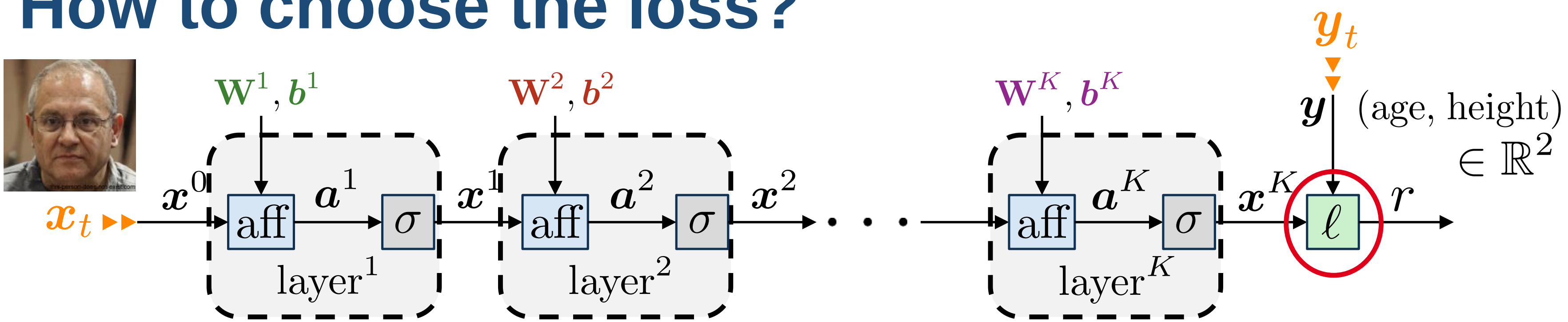

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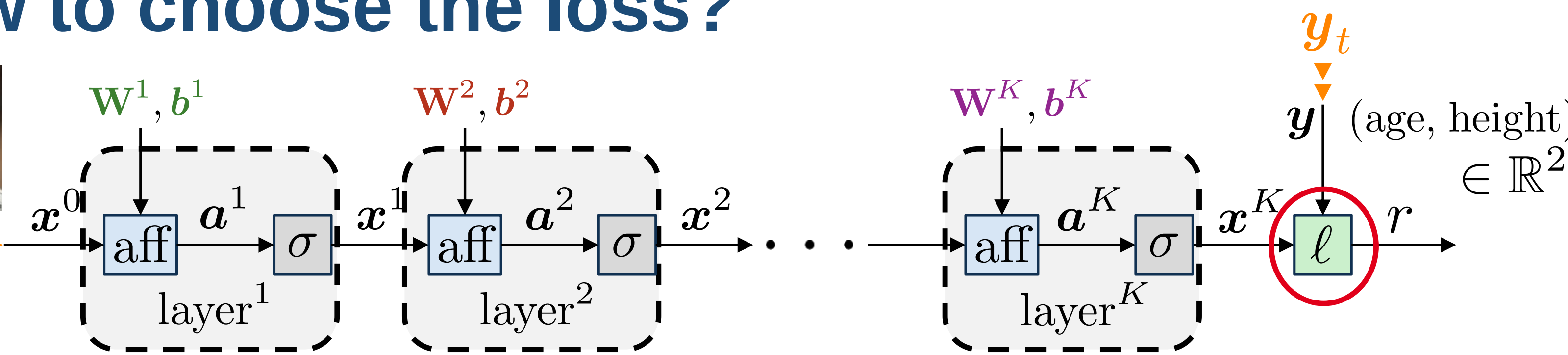

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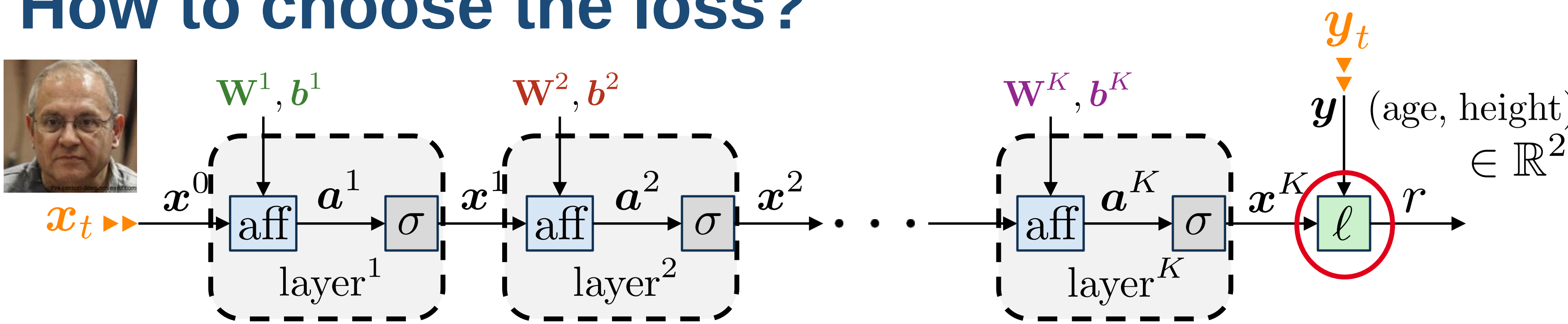

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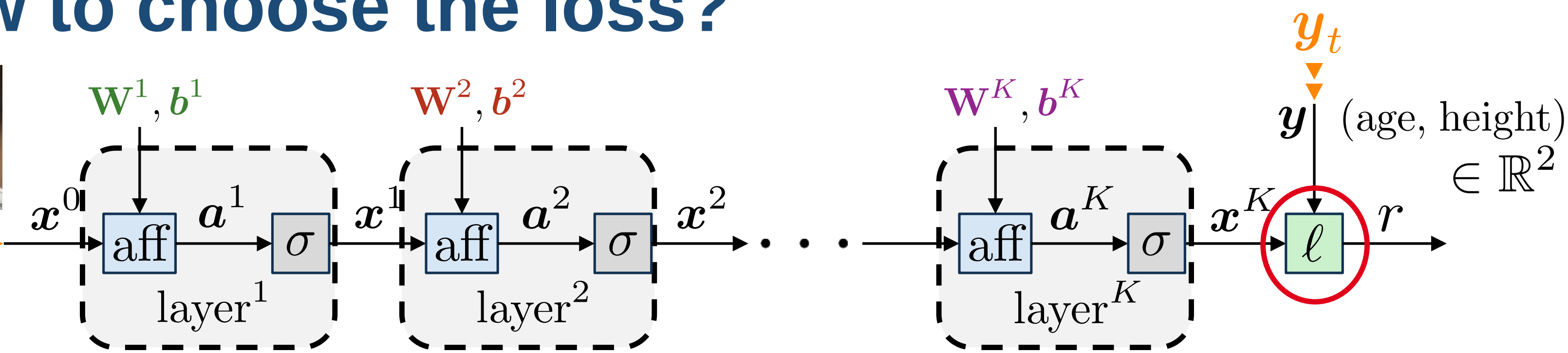

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$\rightarrow$ We recover the **L2 loss**!

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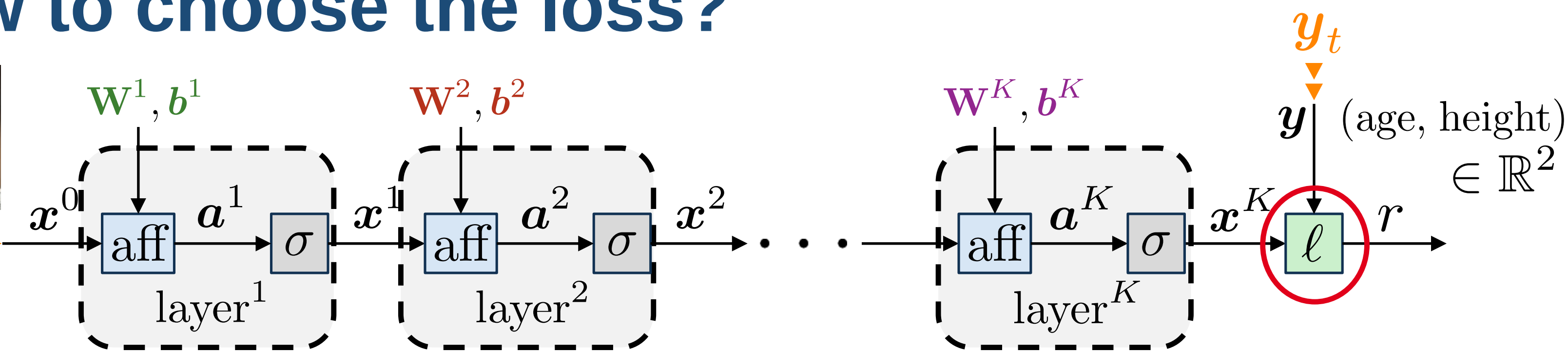

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Using the L2 loss is equivalent to assuming the network will make i.i.d Gaussian errors.

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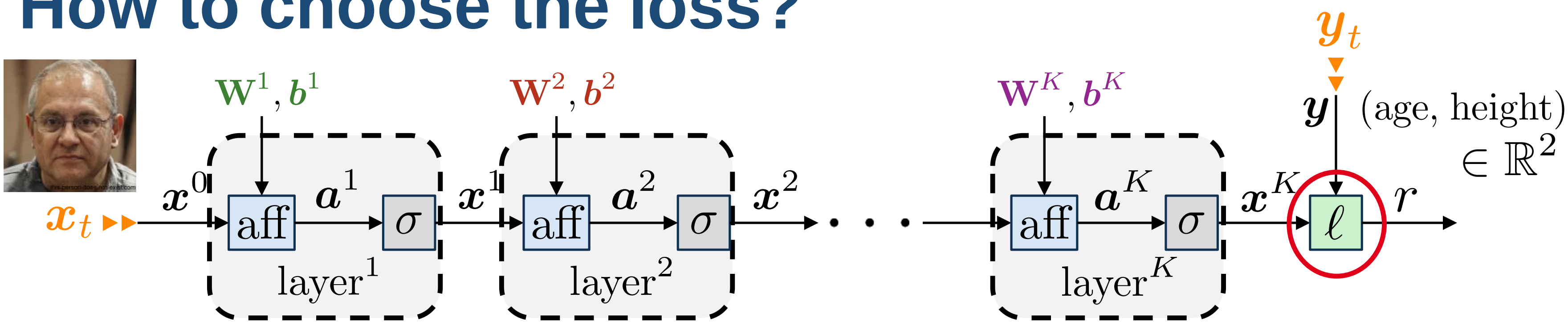

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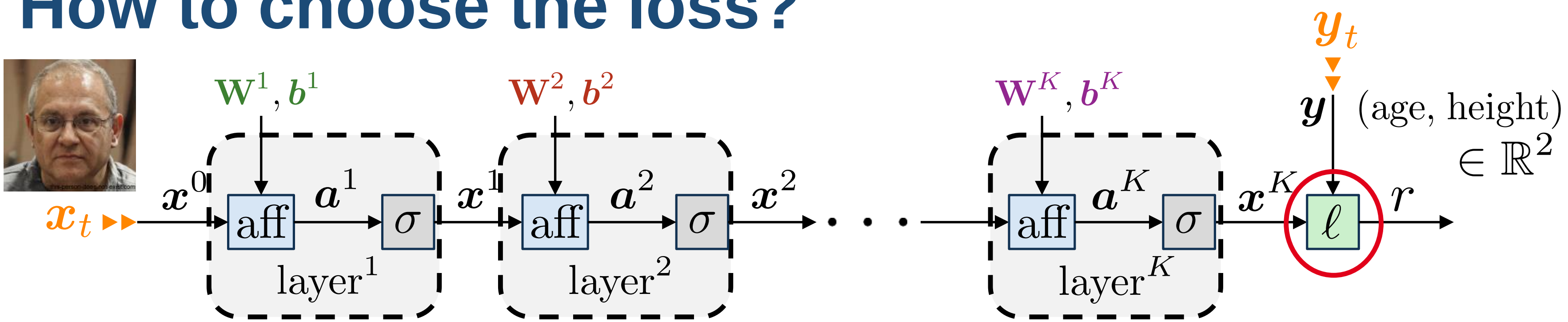

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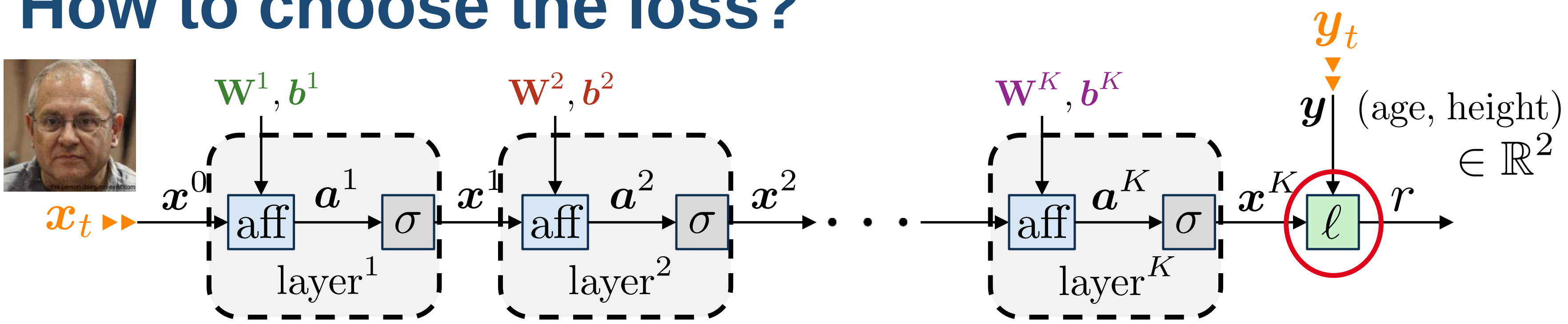

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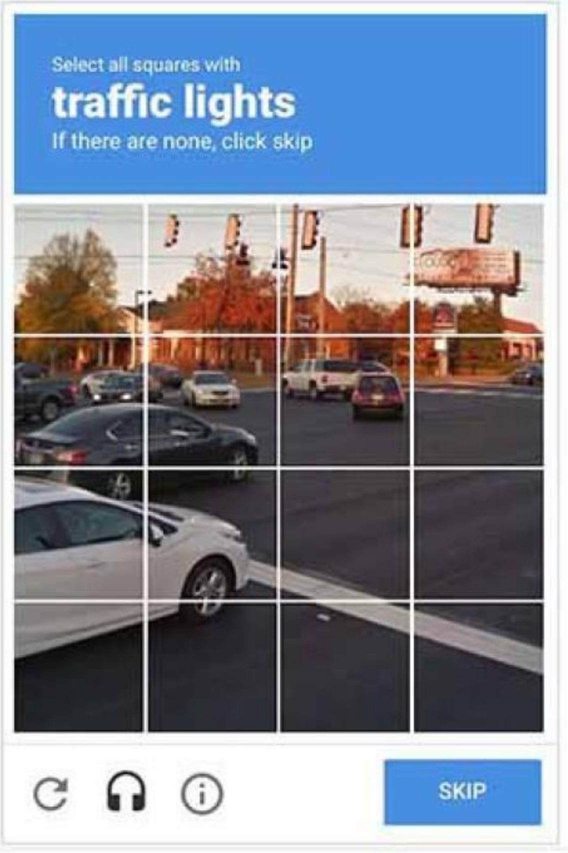
- For $y \geq 0$ we can use an exponential distribution $\tilde{p}_\lambda(y) = \lambda \exp(-\lambda y)$
- We can use this approach to not only estimate **the mean** but also ***the variance*** (≈uncertainty) of the network output:

$$\tilde{p}_{\boldsymbol{\mu},\sigma^2}(\boldsymbol{y}) = \frac{1}{\sqrt{2\pi\sigma^{2N}}} \exp\left(-\frac{\|\boldsymbol{y}-\boldsymbol{\mu}\|_2^2}{2\sigma^2}\right), \quad \boldsymbol{x}^K \equiv [\boldsymbol{\mu}, \sigma^2]$$

Detection

Example: Captcha $\boldsymbol{x}_t \in \mathbb{R}^D, \; y_t \in \{0, 1\}$



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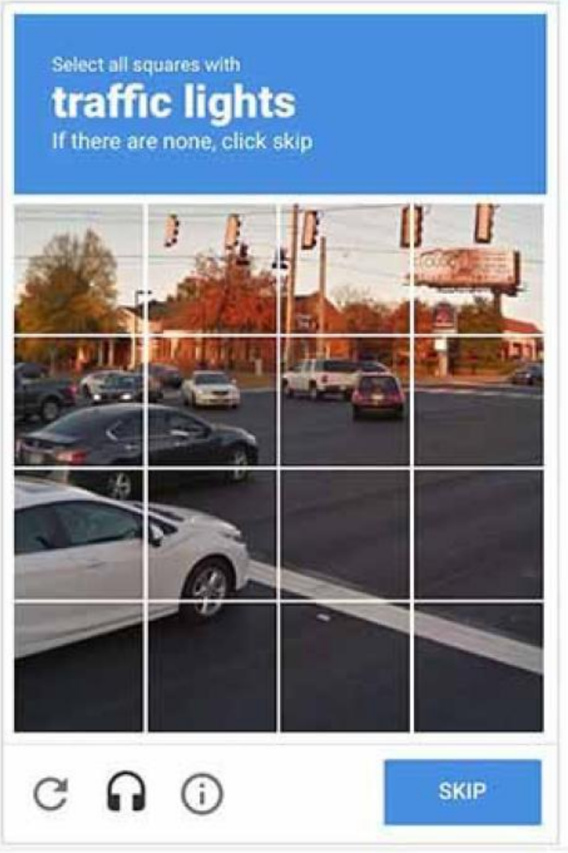

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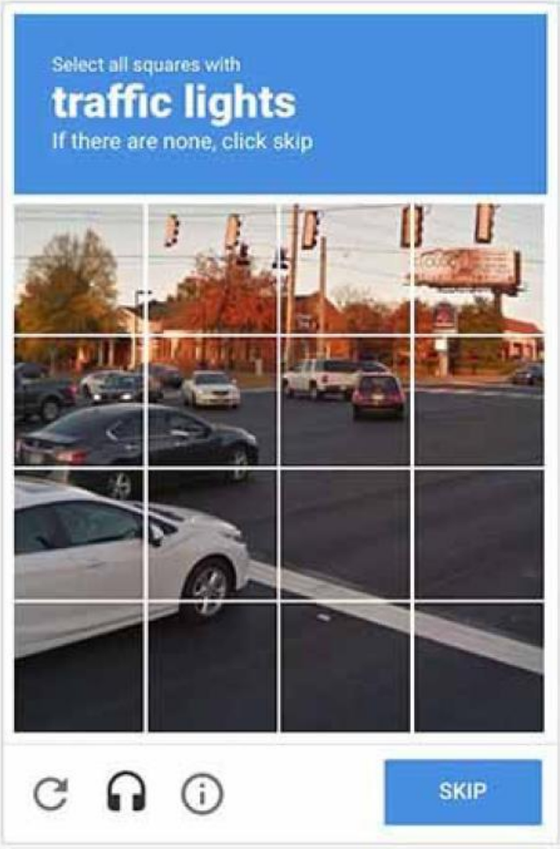

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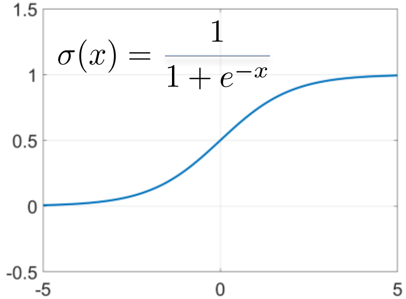

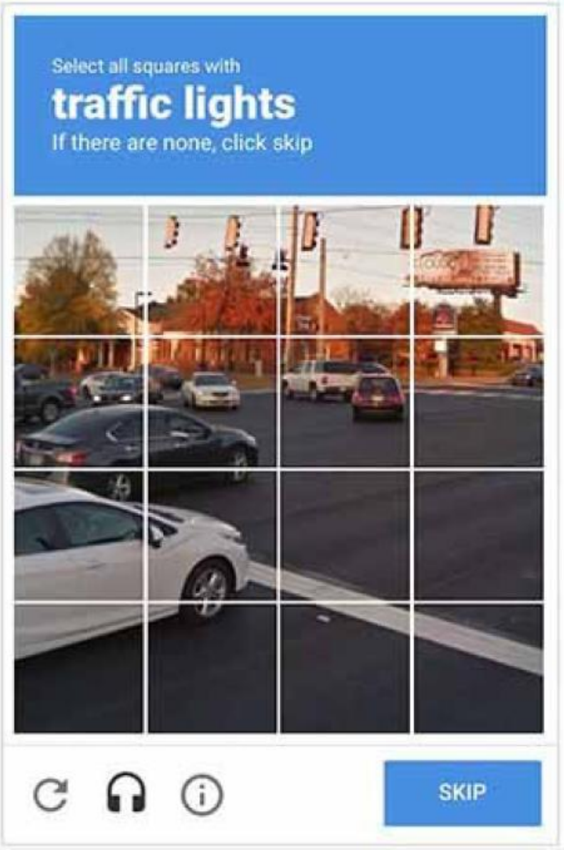

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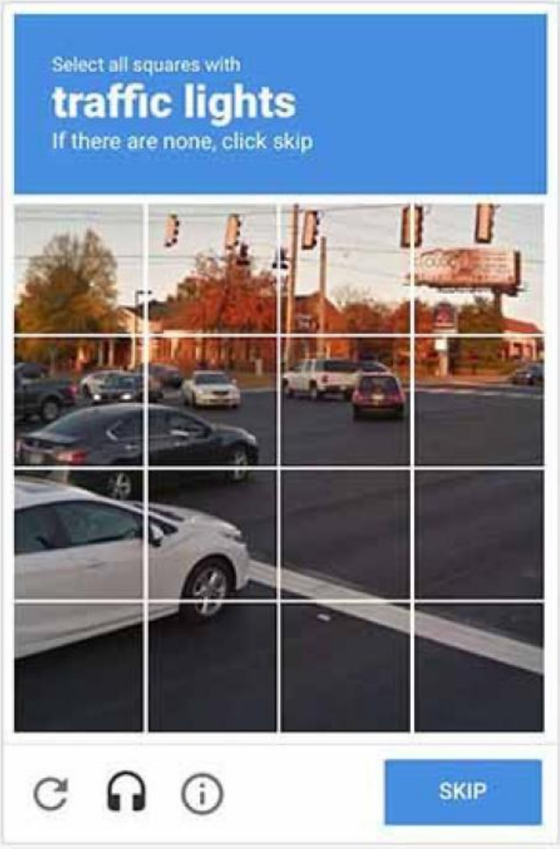

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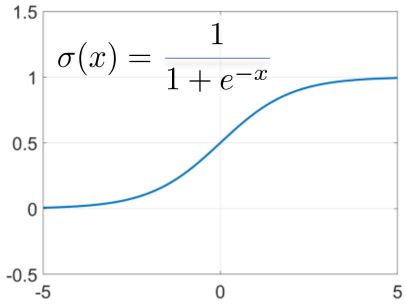

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= the ***Binary Cross-Entropy***.

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- This generalizes to **multi-class classification**

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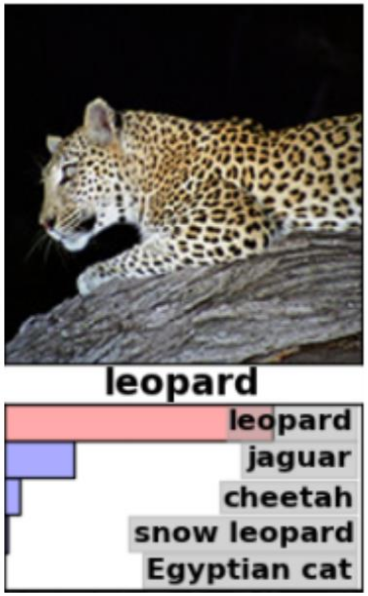

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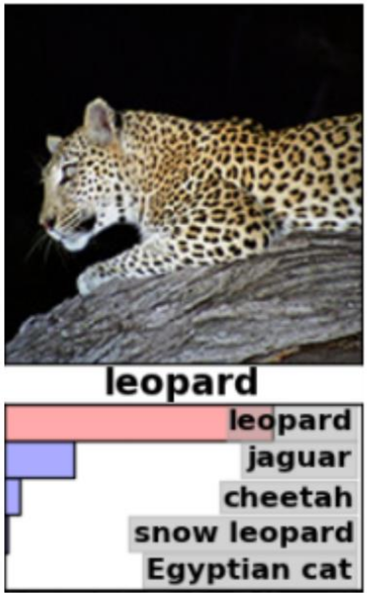

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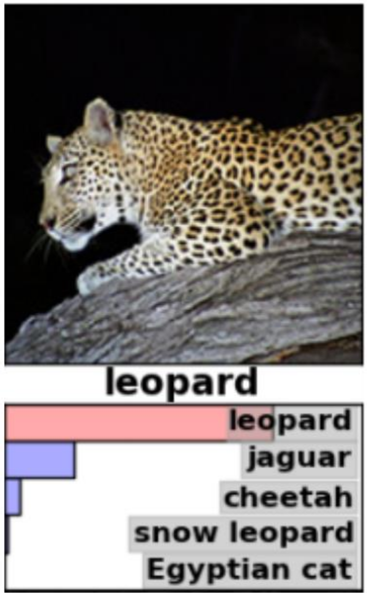

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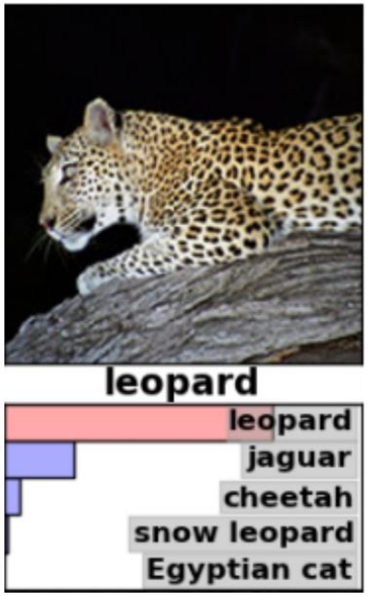

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- Can be done by statistically aggregating **multiple binary detectors**

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$$\ell(\boldsymbol{x}_t^K, \boldsymbol{y}_t) = -\log \tilde{p}_{\boldsymbol{x}_t^K}(\boldsymbol{y}_t) = \sum_{n=1}^{N} -y_{t,n} \log x_{t,n}^K$$

Multi-Label Classification

- Can be done by statistically aggregating **multiple binary detectors**
- Falls in the category of **ensemble methods**

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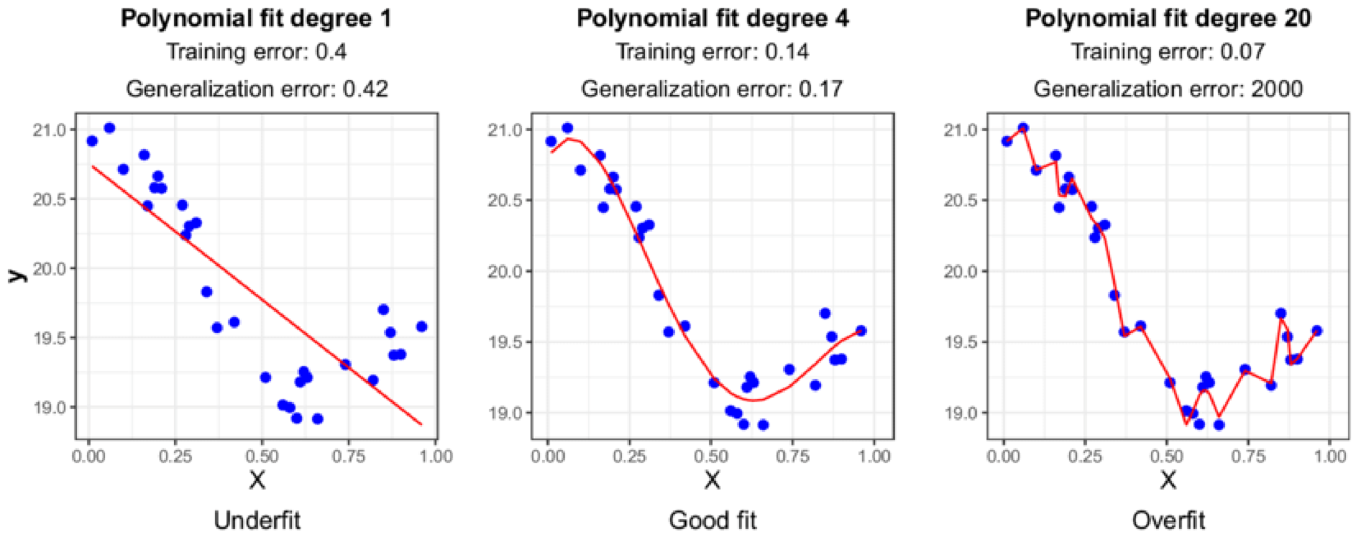
- This may even happen for models of relatively small capacity, if the **amount of training data** is insufficient.

Overfitting

- Ex: polynomial regression



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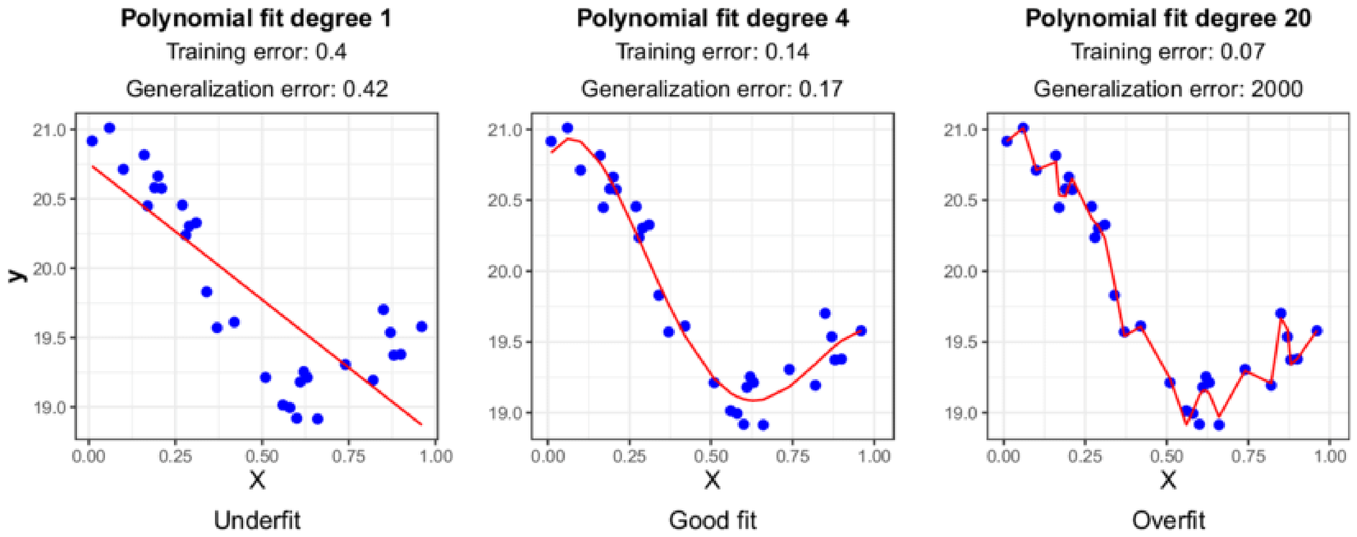
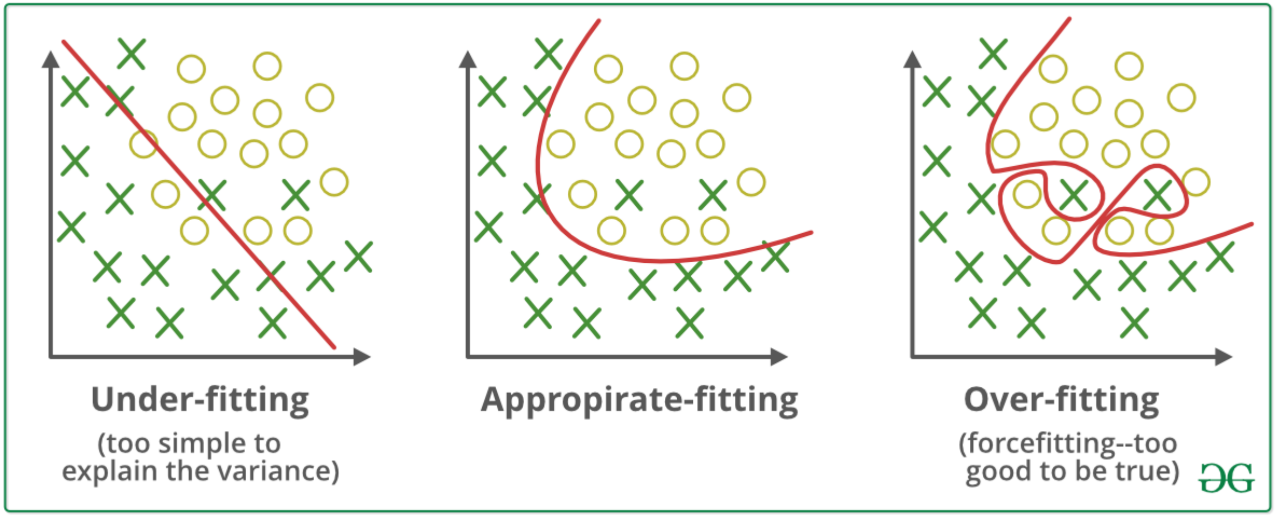


- Ex: binary classification



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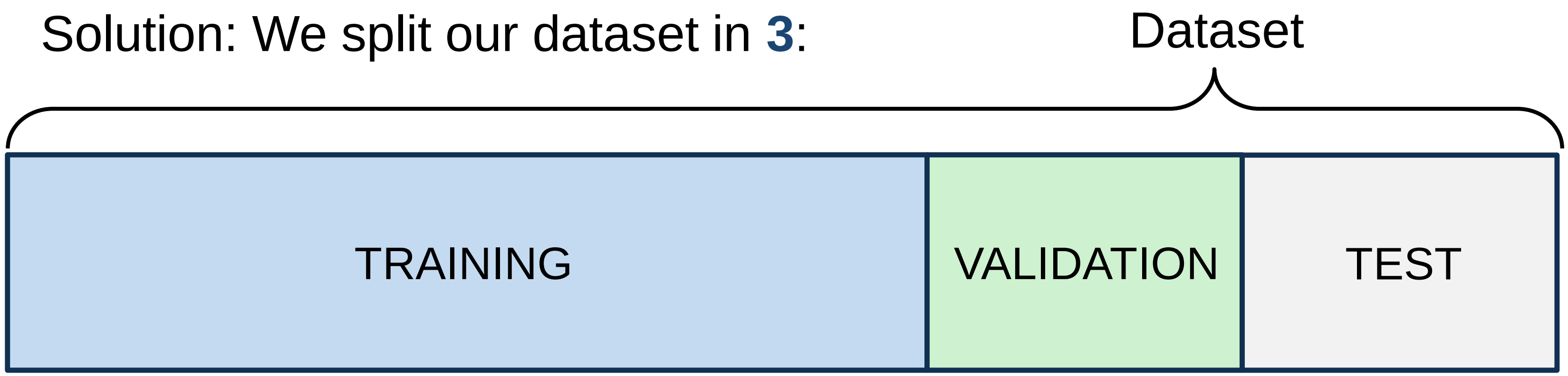

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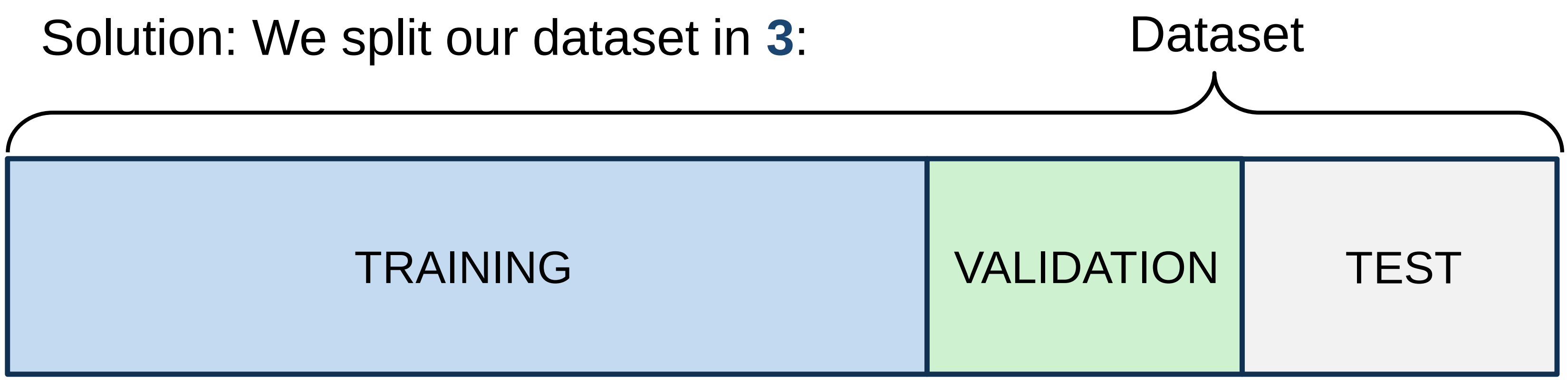

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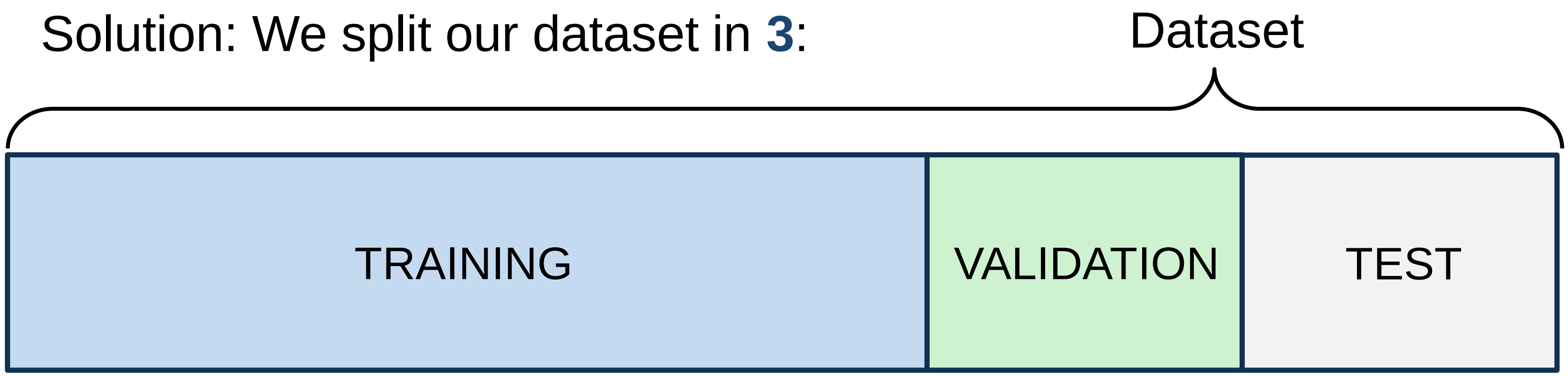

- These 3 subsets must be **perfectly disjoint** and all **representative** of the data.
- To achieve this, the split is done **at random**.

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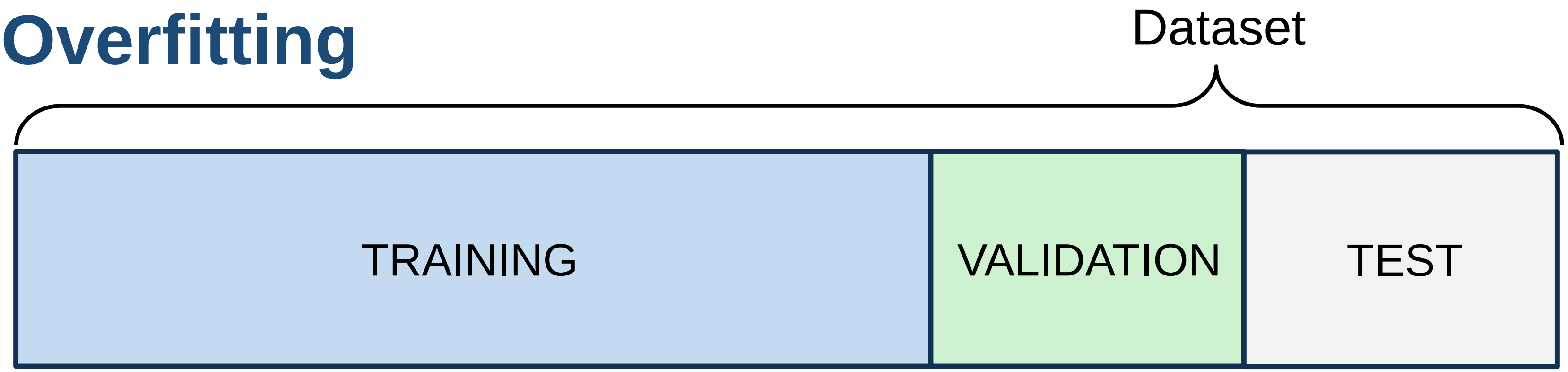

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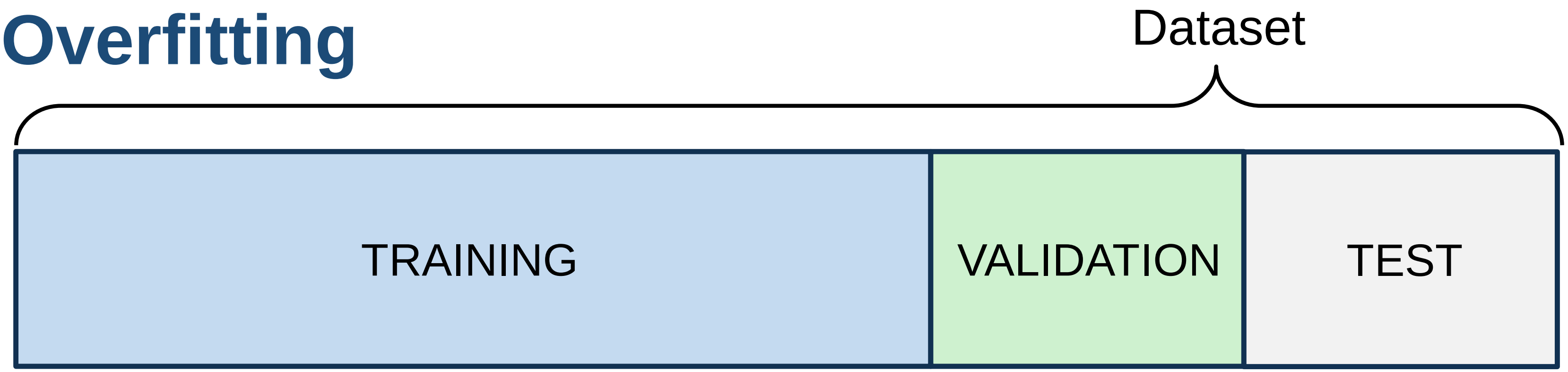

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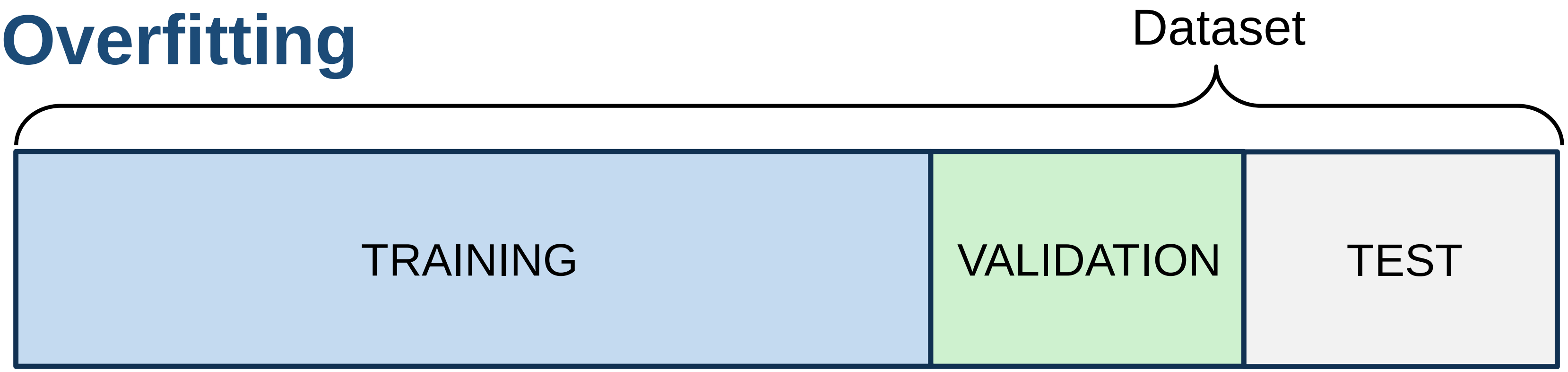

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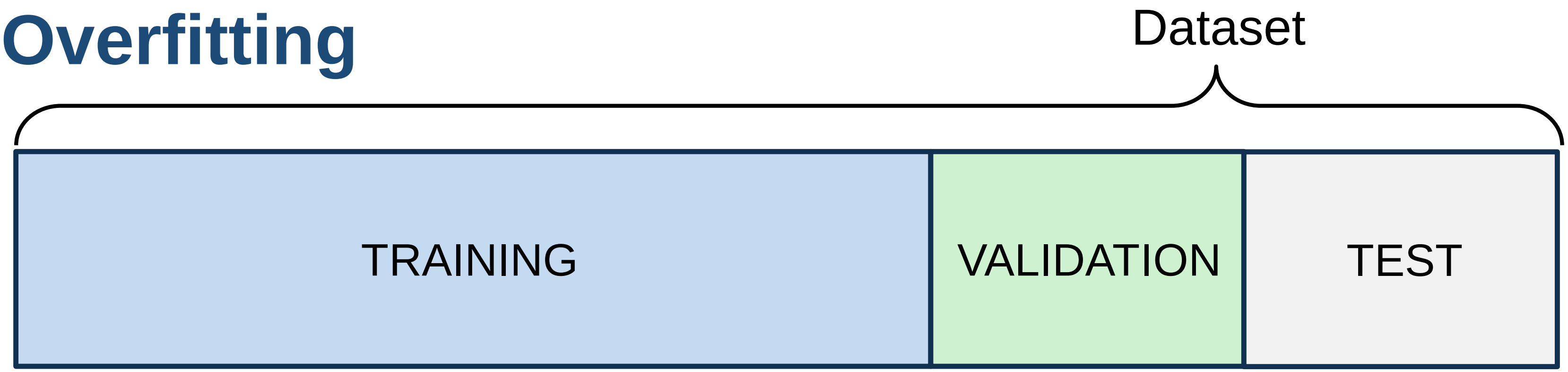

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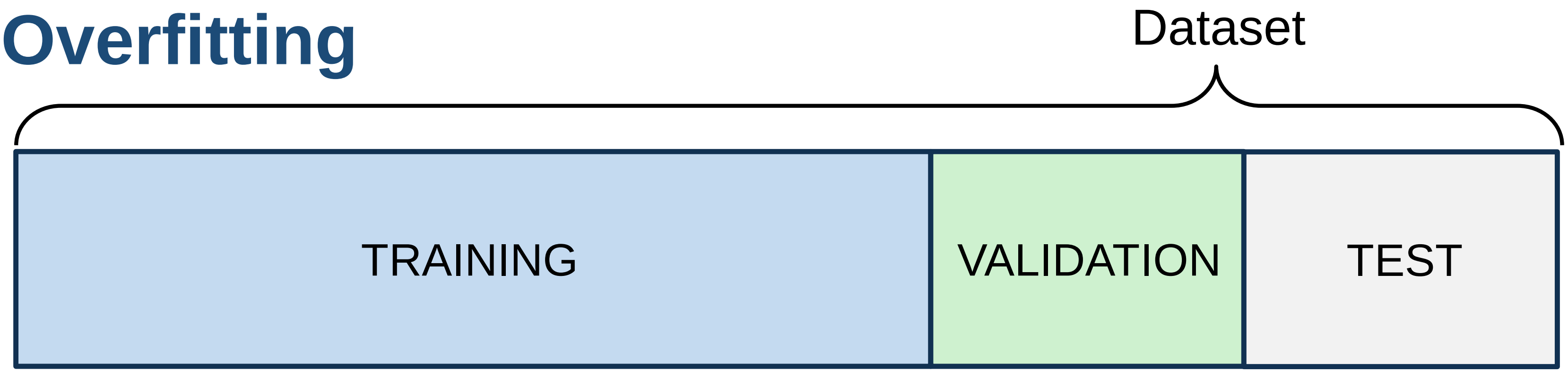

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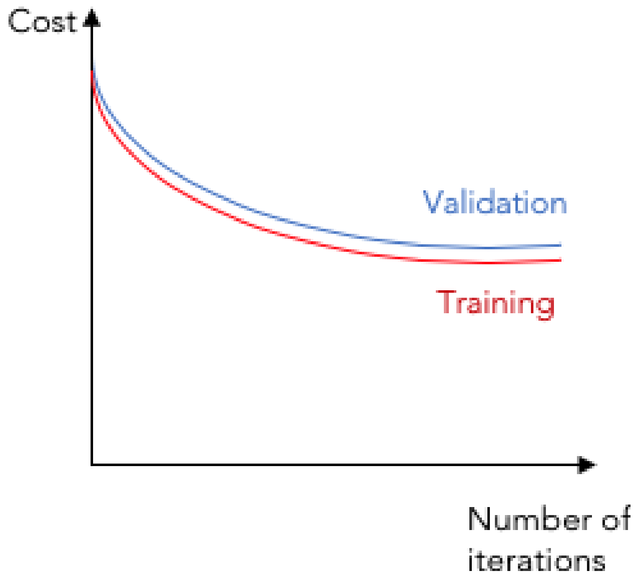
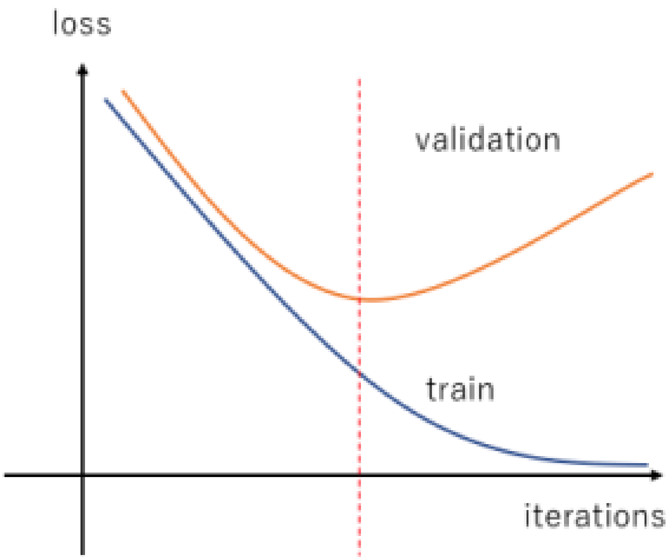
  - Tune hyperparameters (e.g. gradient steps), compare different families of models
- Looking at the test set if **forbidden** in any of those steps *("inverse crime")*

Overfitting

- We can detect overfitting by tracking the **total loss** over the training iterations / epochs:





GOOD. The validation loss is only slightly less good than the training one and does not increase

NOT GOOD. The validation loss increases: we are starting to learn by heart the training set !

Some vocabulary

- **Capacity:** flexibility of a model. It often (but not necessarily!) correlates with the number of parameters of the model
- **Hyper-parameter:** a parameter of a model that is not trained (specified before training)
- **Model selection:** process of choosing the best hyperparameters on the validation set
- **Underfitting:** state of model which could improve generalization with **more** training or **more** capacity
- **Overfitting:** state of model which could improve generalization with **less** training or **less** capacity

Overfitting vs. Underfitting

Quizz

- If capacity increases:
  - training error will ?
  - validation error will ?

- If training time increases:
  - training error will ?
  - validation error will ?

- If training set size increases:
  - generalization error will ?
  - difference between the training and generalization error will ?

Quizz

- If capacity increases:
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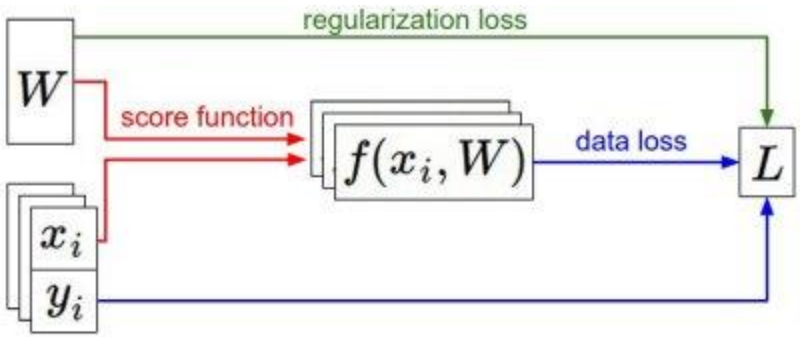
$$L(\mathrm{dnn}_{\boldsymbol{\theta}}, \mathcal{T}) = \frac{1}{T}\sum_{t=1}^{T} \ell\left(\mathrm{dnn}_{\boldsymbol{\theta}}(\boldsymbol{x}_t), \boldsymbol{y}_t\right) + \lambda\mathcal{R}(\boldsymbol{\theta})$$



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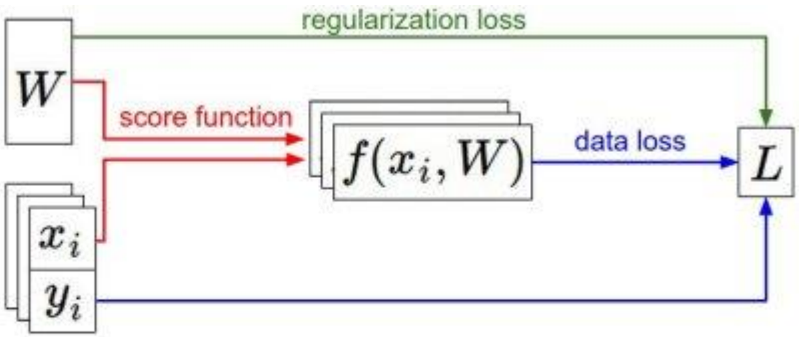
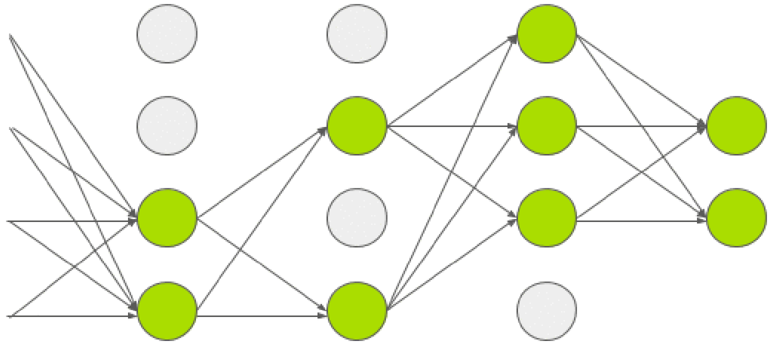


- For example, we could add the **L2 norm** of the coefficients in the **weight matrices**, to avoid that they become very large (a common clue of overfitting)

Techniques to reduce overfitting

2) Dropout



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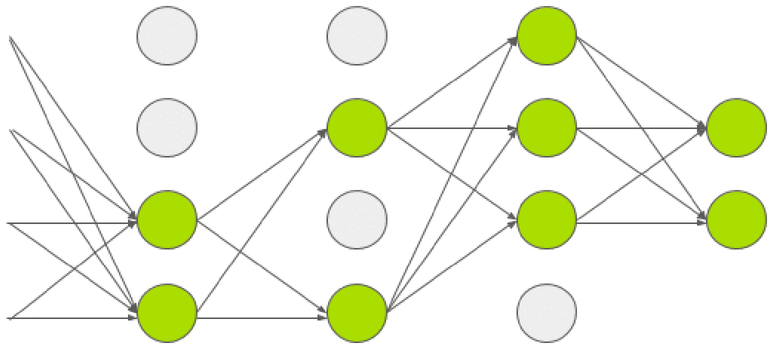

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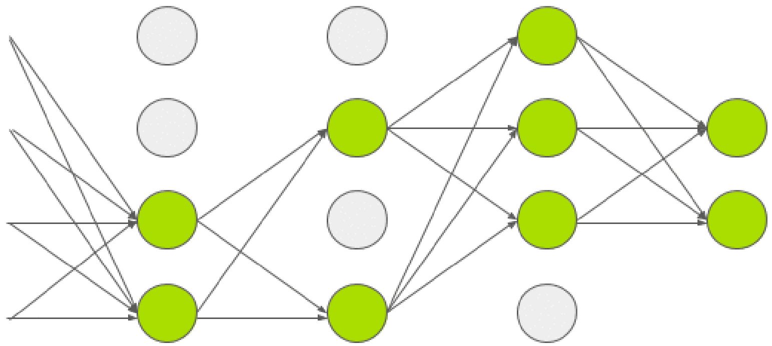

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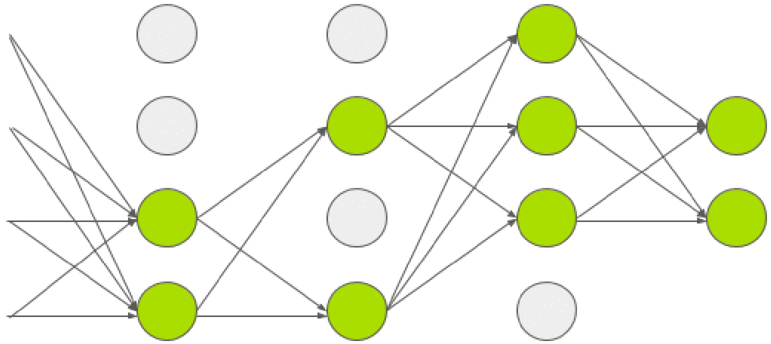

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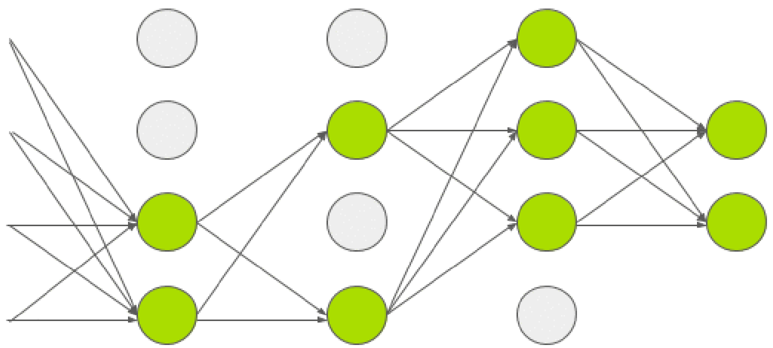

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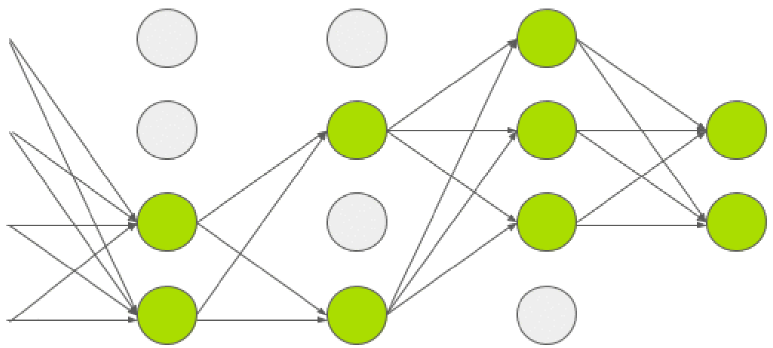

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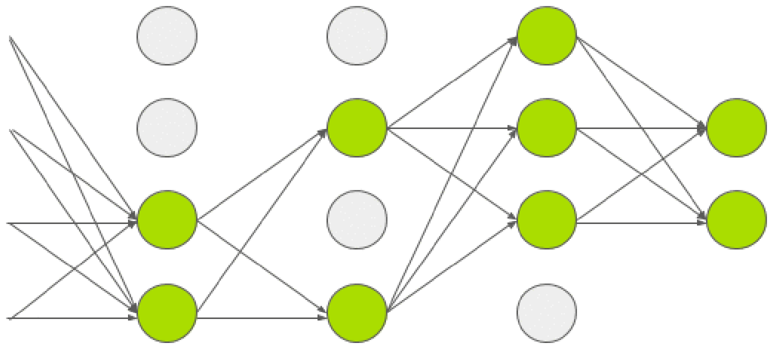

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- Can be viewed as averaging an exponential number of networks.

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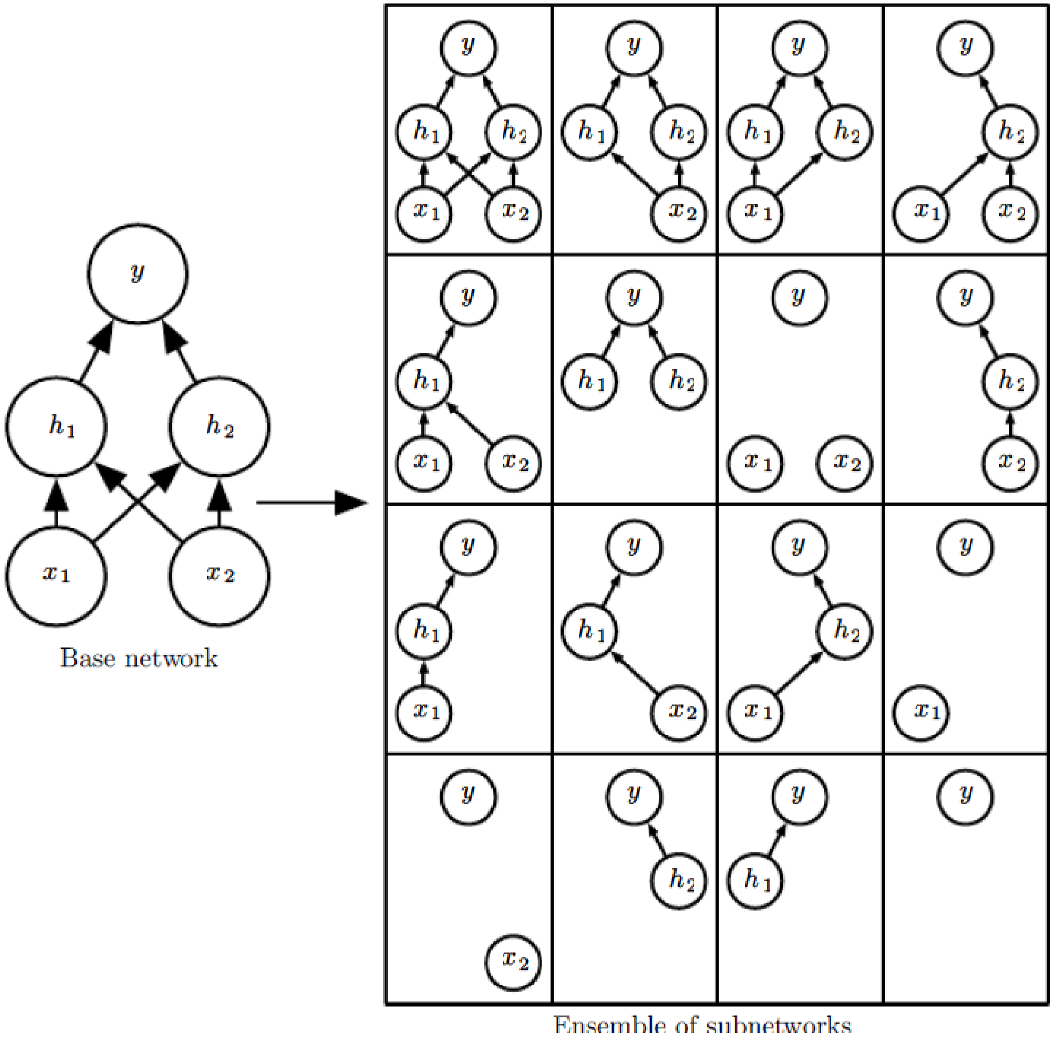

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- Data augmentation is often key for a ML method to work

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