6.867 Machine learning: lecture 2

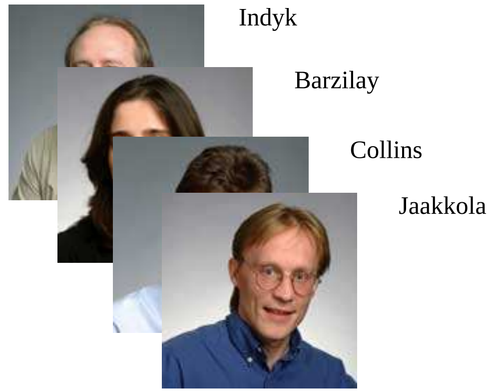
Tommi S. Jaakkola
MIT CSAIL
tommi@csail.mit.edu

Topics

- The learning problem
  - hypothesis class, estimation algorithm
  - loss and estimation criterion
  - sampling, empirical and expected losses
- Regression, example
- Linear regression
  - estimation, errors, analysis

Review: the learning problem

- Recall the image (face) recognition problem



- **Hypothesis class**: we consider some *restricted* set $\mathcal{F}$ of mappings $f : \mathcal{X} \rightarrow \mathcal{L}$ from images to labels
- **Estimation:** on the basis of a training set of examples and labels, $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$, we find an estimate $\hat{f} \in \mathcal{F}$
- **Evaluation:** we measure how well $\hat{f}$ *generalizes* to yet unseen examples, i.e., whether $\hat{f}(\mathbf{x}_{new})$ agrees with y_{new}

Hypotheses and estimation

- We used a simple linear classifier, a parameterized mapping $f(\mathbf{x};\theta)$ from images $\mathcal{X}$ to labels $\mathcal{L}$, to solve a binary image classification problem (2's vs 3's):

$$\hat{y} \;=\; f(\mathbf{x};\theta) = \text{sign}\big(\,\theta\cdot\mathbf{x}\,\big)$$

  where $\mathbf{x}$ is a pixel image and $\hat{y} \in \{-1, 1\}$.

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where $\mathbf{x}$ is a pixel image and $\hat{y} \in \{-1, 1\}$.

- The parameters θ were adjusted on the basis of the training examples and labels according to a simple mistake driven update rule (written here in a vector form)

$$\theta \leftarrow \theta + y_i \mathbf{x}_i, \quad \text{whenever} \quad y_i \neq \text{sign}\big(\,\theta \cdot \mathbf{x}_i\,\big)$$

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- The update rule attempts to minimize the number of errors that the classifier makes on the training examples

Estimation criterion

- We can formulate the estimation problem more explicitly by defining a *zero-one loss*:

$$\text{Loss}(y, \hat{y}) = \begin{cases} 0, y = \hat{y} \\ 1, y \neq \hat{y} \end{cases}$$

so that

$$\frac{1}{n} \sum_{i=1}^{n} \text{Loss}(y_i, \hat{y}_i) = \frac{1}{n} \sum_{i=1}^{n} \text{Loss}(y_i, f(\mathbf{x}_i; \theta))$$

gives the fraction of prediction errors on the training set.

- This is a function of the parameters θ and we can try to minimize it directly.

Estimation criterion cont'd

- We have reduced the estimation problem to a minimization problem

$$\text{find } \theta \text{ that minimizes} \qquad \overbrace{\frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, f(\mathbf{x}_i;\theta)\big)}^{\text{empirical loss}}$$

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  – valid when the predictions are discrete labels, real valued, or other provided that the loss is defined appropriately
  – may be ill-posed (under-constrained) as stated

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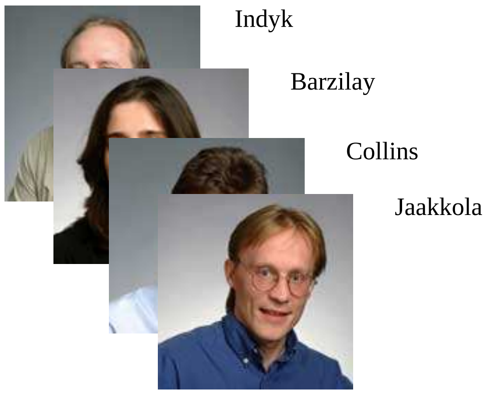
- But why is it sensible to minimize the *empirical loss* in the first place since we are only interested in the performance on new examples?

Training and test performance: sampling

- We assume that each training *and* test example-label pair, $(\mathbf{x}, y)$, is drawn *independently at random* from the *same* but unknown population of examples and labels.

- We can represent this population as a joint probability distribution $P(\mathbf{x}, y)$ so that each training/test example is a *sample* from this distribution $(\mathbf{x}_i, y_i) \sim P$



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$$\text{Empirical (training) loss} \;=\; \frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, f(\mathbf{x}_i;\theta)\big)$$

$$\text{Expected (test) loss} \;=\; E_{(\mathbf{x},y)\sim P}\left\{\text{Loss}\big(y, f(\mathbf{x};\theta)\big)\right\}$$

- The training loss based on a few sampled examples and labels serves as a proxy for the test performance measured over the whole population.

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Regression

- The goal is to make quantitative (real valued) predictions on the basis of a (vector of) features or attributes
- Example: predicting vehicle fuel efficiency (mpg) from 8 attributes

y			$\mathbf{x}$		
	cyls	disp	hp	weight	...
18.0	8	307.0	130.00	3504	...
26.0	4	97.00	46.00	1835	...
33.5	4	98.00	83.00	2075	...
...					

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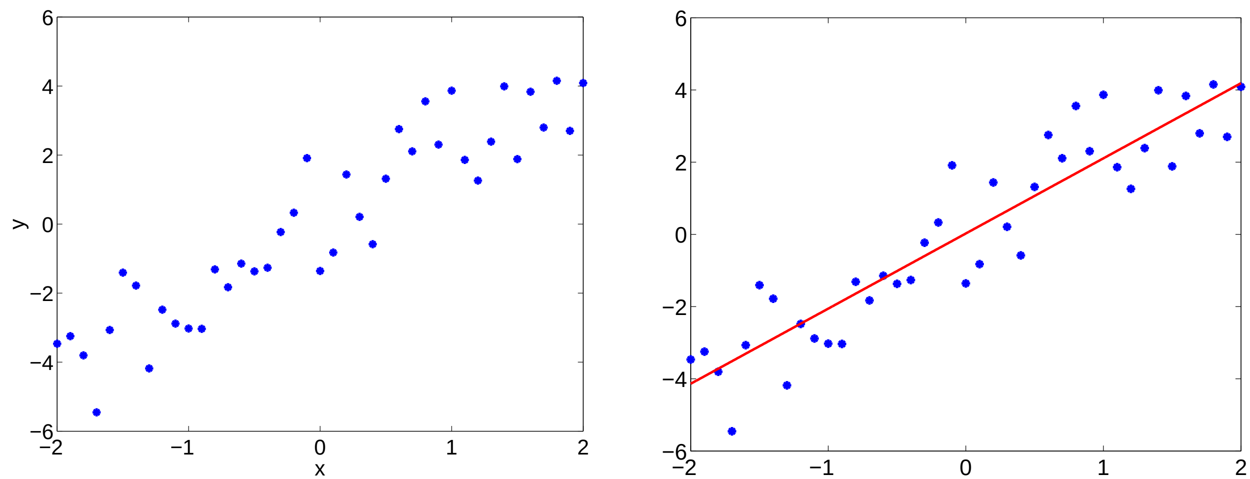
...					

- We need to
  - specify the class of functions (e.g., linear)
  - select how to measure prediction loss
  - solve the resulting minimization problem

Linear regression



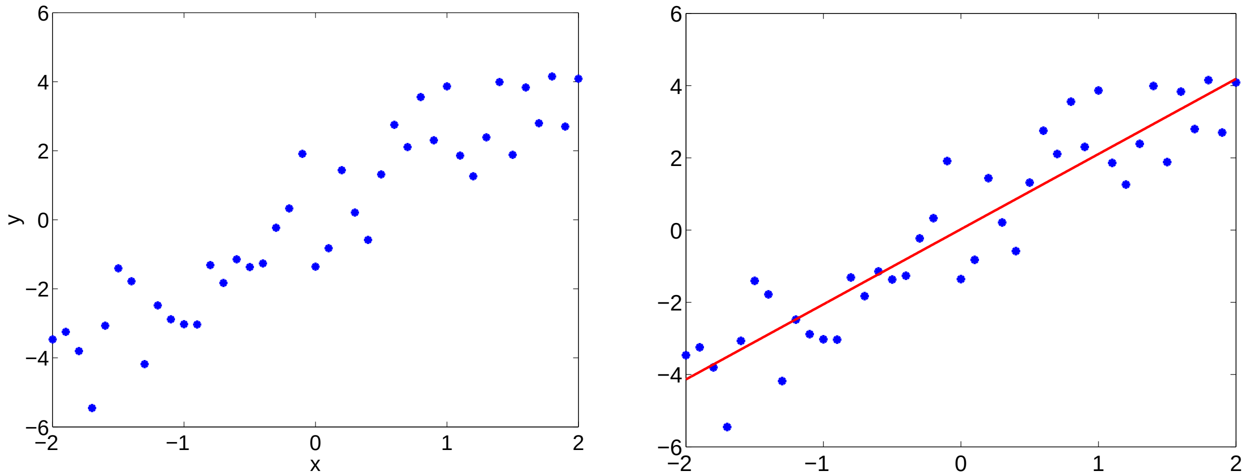
- We begin by considering linear regression (easy to extend to more complex predictions later on)

$$f : \mathcal{R} \rightarrow \mathcal{R} \qquad f(x; \mathbf{w}) = w_0 + w_1 x$$

$$f : \mathcal{R}^d \rightarrow \mathcal{R} \qquad f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

where $\mathbf{w} = [w_0, w_1, \ldots, w_d]^T$ are *parameters* we need to set.

Linear regression: squared loss



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$$f : \mathcal{R}^d \rightarrow \mathcal{R} \qquad f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

- We can measure the prediction loss in terms of squared error, Loss$(y, \hat{y}) = (y - \hat{y})^2$, so that the empirical loss on n training samples becomes *mean squared error*

$$J_n(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} \big(y_i - f(\mathbf{x}_i; \mathbf{w}) \big)^2$$

Linear regression: estimation

- We have to minimize the *empirical* squared loss

$$
\begin{aligned}
J_n(\mathbf{w}) &= \frac{1}{n}\sum_{i=1}^{n}\big(y_i - f(\mathbf{x}_i;\mathbf{w})\big)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i)^2 \quad \text{(1-dim)}
\end{aligned}
$$

By setting the derivatives with respect to w_1 and w_0 to zero, we get necessary conditions for the "optimal" parameter values

$$
\begin{aligned}
\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= 0 \\
\frac{\partial}{\partial w_0} J_n(\mathbf{w}) &= 0
\end{aligned}
$$

Optimality conditions: derivation

$$\frac{\partial}{\partial w_1} J_n(\mathbf{w}) \;\; = \;\; \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2$$

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&= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i) \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)
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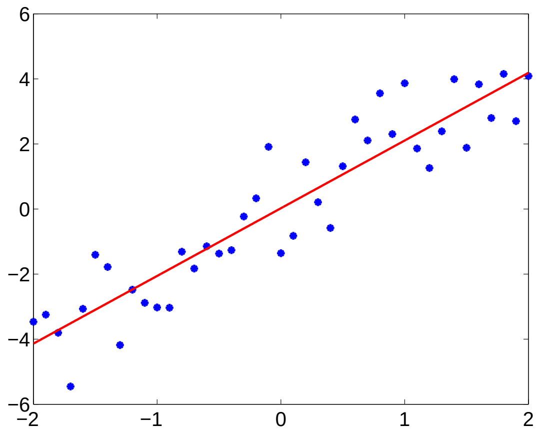
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)(-x_i) = 0 \\
\frac{\partial}{\partial w_0} J_n(\mathbf{w}) &= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)(-1) = 0
\end{aligned}
$$

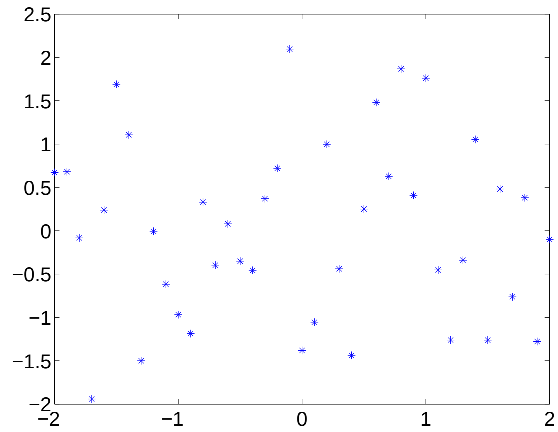
Interpretation

- If we denote the prediction error as $\epsilon_i = (y_i - w_0 - w_1 x_i)$ then the optimality conditions can be written as

$$\frac{1}{n}\sum_{i=1}^{n} \epsilon_i x_i = 0, \quad \frac{1}{n}\sum_{i=1}^{n} \epsilon_i = 0$$

Thus the prediction error is uncorrelated with any linear function of the inputs





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$$\frac{1}{n}\sum_{i=1}^{n} \epsilon_i x_i = 0, \quad \frac{1}{n}\sum_{i=1}^{n} \epsilon_i = 0$$

Thus the prediction error is uncorrelated with any linear function of the inputs

but not with a quadratic function of the inputs

$$\frac{1}{n}\sum_{i=1}^{n} \epsilon_i x_i^2 \neq 0 \quad \text{(in general)}$$

Linear regression: matrix notation

- We can express the solution a bit more generally by resorting to a matrix notation

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \cdots \\ y_n \end{bmatrix}, \; \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \cdots & \cdots \\ 1 & x_n \end{bmatrix}, \; \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

so that

$$\begin{aligned} \frac{1}{n}\sum_{t=1}^{n}(y_t - w_0 - w_1 x_t)^2 &= \frac{1}{n}\left\| \begin{bmatrix} y_1 \\ \cdots \\ y_n \end{bmatrix} - \begin{bmatrix} 1 & x_1 \\ \cdots & \cdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \right\|^2 \\ &= \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \end{aligned}$$

Linear regression: solution

By setting the derivatives of $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2/n$ to zero, we get the same optimality conditions as before, now expressed in a matrix form

$$\frac{\partial}{\partial \mathbf{w}} \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 = \frac{\partial}{\partial \mathbf{w}} \frac{1}{n}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

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\frac{\partial}{\partial \mathbf{w}} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 &= \frac{\partial}{\partial \mathbf{w}} \frac{1}{n} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= \frac{2}{n} \mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w})
\end{aligned}
$$

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&= \frac{2}{n} \mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= \frac{2}{n} (\mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X}\mathbf{w}) = \mathbf{0}
\end{aligned}
$$

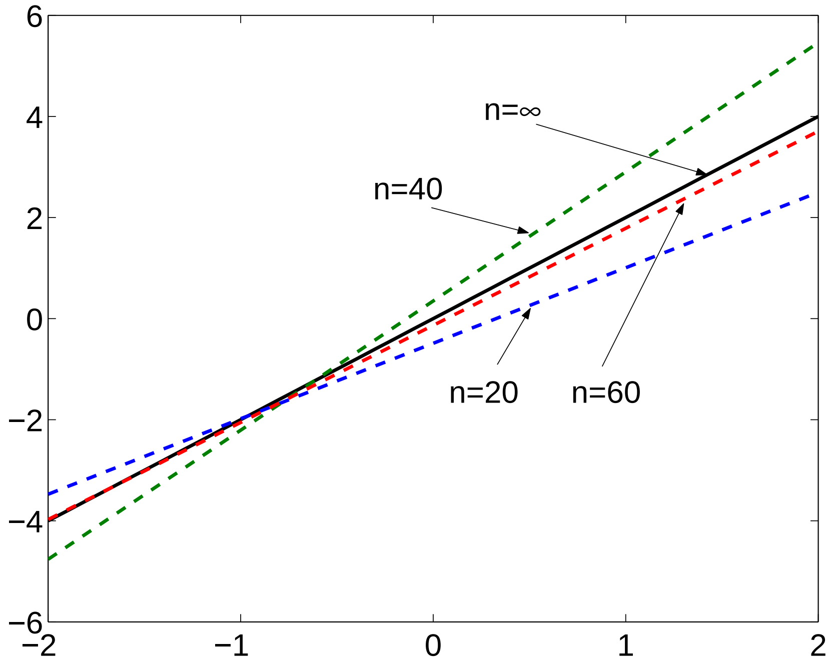
which gives

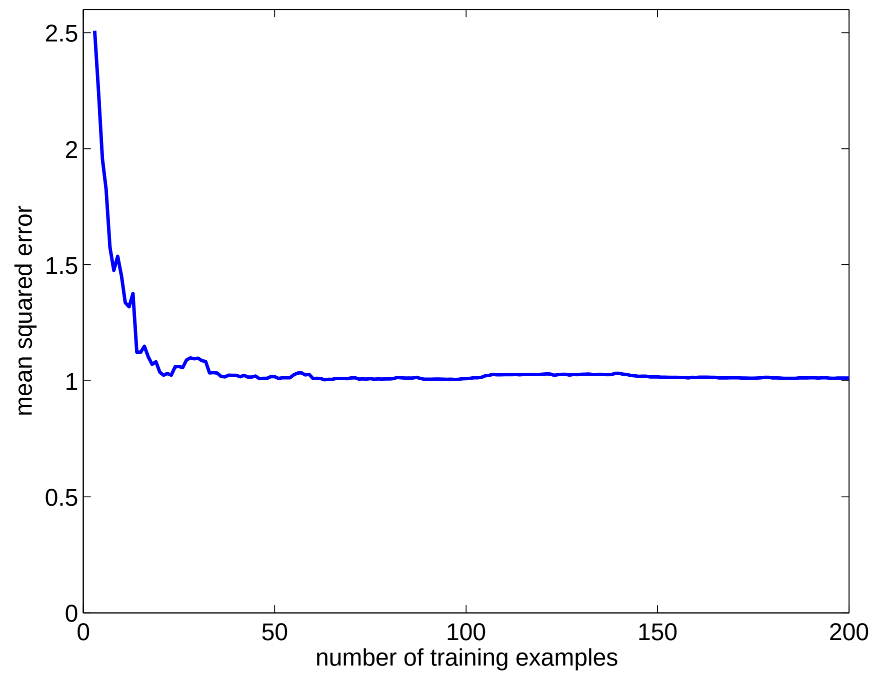
$$\hat{\mathbf{w}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

- The solution is a linear function of the outputs y

Linear regression: generalization

- As the number of training examples increases our solution gets "better"





We'd like to understand the error a bit better

Linear regression: types of errors

- Structural error measures the error introduced by the limited function class (infinite training data):

$$\min_{w_1, w_0} E_{(x,y)\sim P} \left(y - w_0 - w_1 x\right)^2 = E_{(x,y)\sim P} \left(y - w_0^* - w_1^* x\right)^2$$

where (w_0^*, w_1^*) are the optimal linear regression parameters.

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where (w_0^*, w_1^*) are the optimal linear regression parameters.

- Approximation error measures how close we can get to the optimal linear predictions with limited training data:

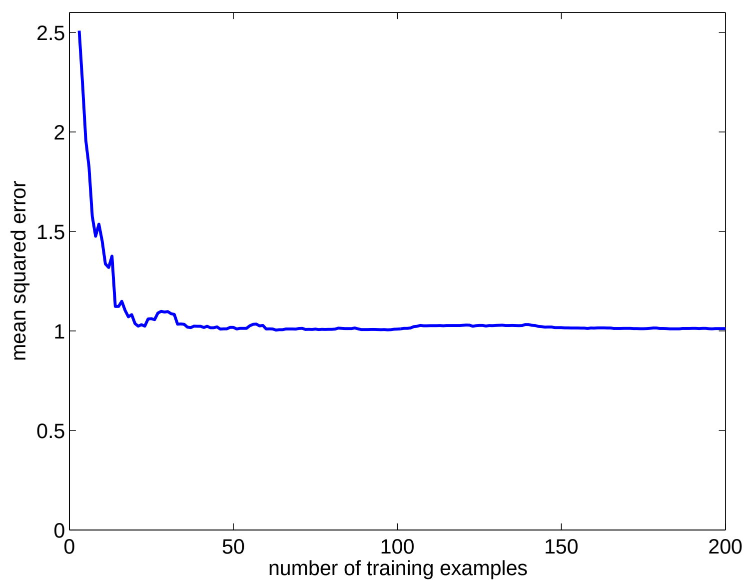
$$E_{(x,y)\sim P}\,(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x)^2$$

where $(\hat{w}_0, \hat{w}_1)$ are the parameter estimates based on a small training set (therefore themselves random variables).

Linear regression: error decomposition

- The expected error of our linear regression function decomposes into the sum of structural and approximation errors

$$
\begin{aligned}
E_{(x,y)\sim P}\left(y - \hat{w}_0 - \hat{w}_1 x\right)^2 = \\
& E_{(x,y)\sim P}\left(y - w_0^* - w_1^* x\right)^2 + \\
& E_{(x,y)\sim P}\left(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x\right)^2
\end{aligned}
$$



Error decomposition: derivation

$$
\begin{aligned}
& E_{(x,y)\sim P}\,(y - \hat{w}_0 - \hat{w}_1 x)^2 \\
&\quad = \; E_{(x,y)\sim P}\left((y - w_0^* - w_1^* x) + (w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x)\right)^2 \\
&\quad = \; E_{(x,y)\sim P}\,(y - w_0^* - w_1^* x)^2 \\
&\qquad\quad + E_{(x,y)\sim P}\, 2(y - w_0^* - w_1^* x)(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x) \\
&\qquad\quad + E_{(x,y)\sim P}\,(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x)^2
\end{aligned}
$$

The second term has to be zero since the error $(y - w_0^* - w_1^* x)$ of the best linear predictor is necessarily uncorrelated with any linear function of the input including $(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x)$