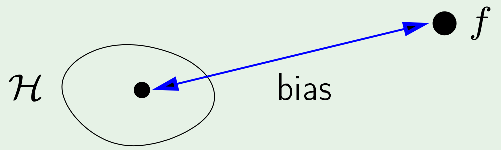
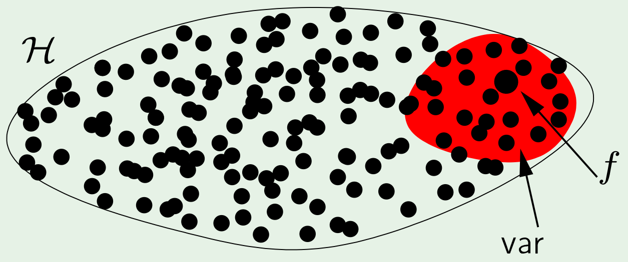
Review of Lecture 8

- Bias and variance

Expected value of E_{out} w.r.t. $\mathcal{D}$

$$= \text{bias} + \text{var}$$



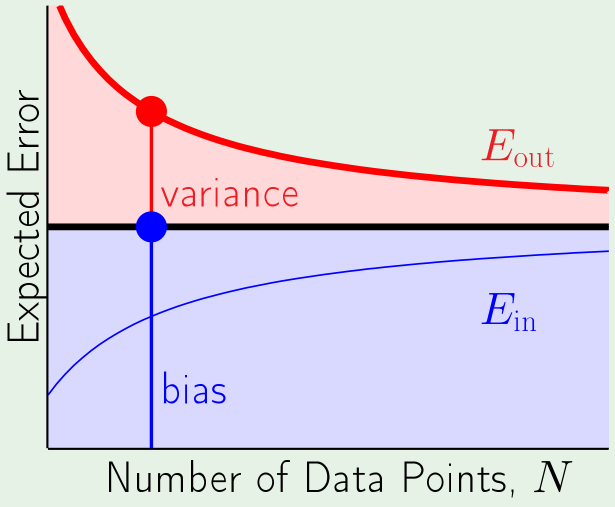


$$g^{(\mathcal{D})}(\mathbf{x}) \rightarrow \bar{g}(\mathbf{x}) \rightarrow f(\mathbf{x})$$

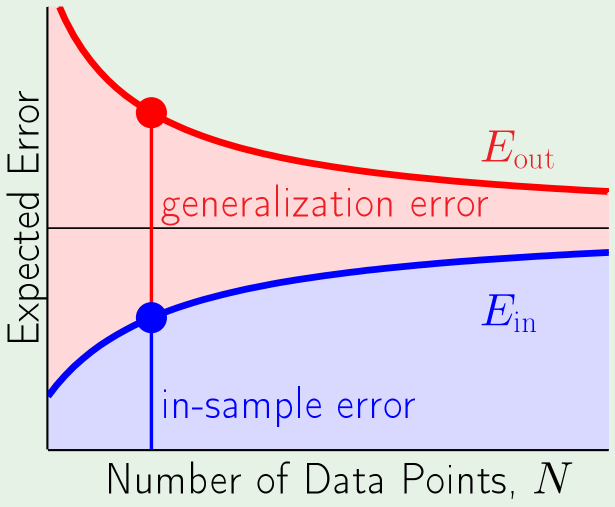
- Learning curves

How E_{in} and E_{out} vary with N

B-V:



VC:



- $N \propto$ "VC dimension"

Learning From Data

Yaser S. Abu-Mostafa
California Institute of Technology

Lecture 9: The Linear Model II

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 1, 2012

Where we are

- Linear classification ✓
- Linear regression ✓
- Logistic regression
- Nonlinear transforms $\approx$✓

Nonlinear transforms

$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \quad \xrightarrow{\Phi} \quad \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots\cdots, z_{\tilde{d}})$$

Each $z_i = \phi_i(\mathbf{x})$ $\qquad$ $\mathbf{z} = \Phi(\mathbf{x})$

Example: $\mathbf{z} = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$

Final hypothesis $g(\mathbf{x})$ in $\mathcal{X}$ space:

$\operatorname{sign}\left(\tilde{\mathbf{w}}^{\mathsf{T}}\Phi(\mathbf{x})\right)$ or $\tilde{\mathbf{w}}^{\mathsf{T}}\Phi(\mathbf{x})$

The price we pay

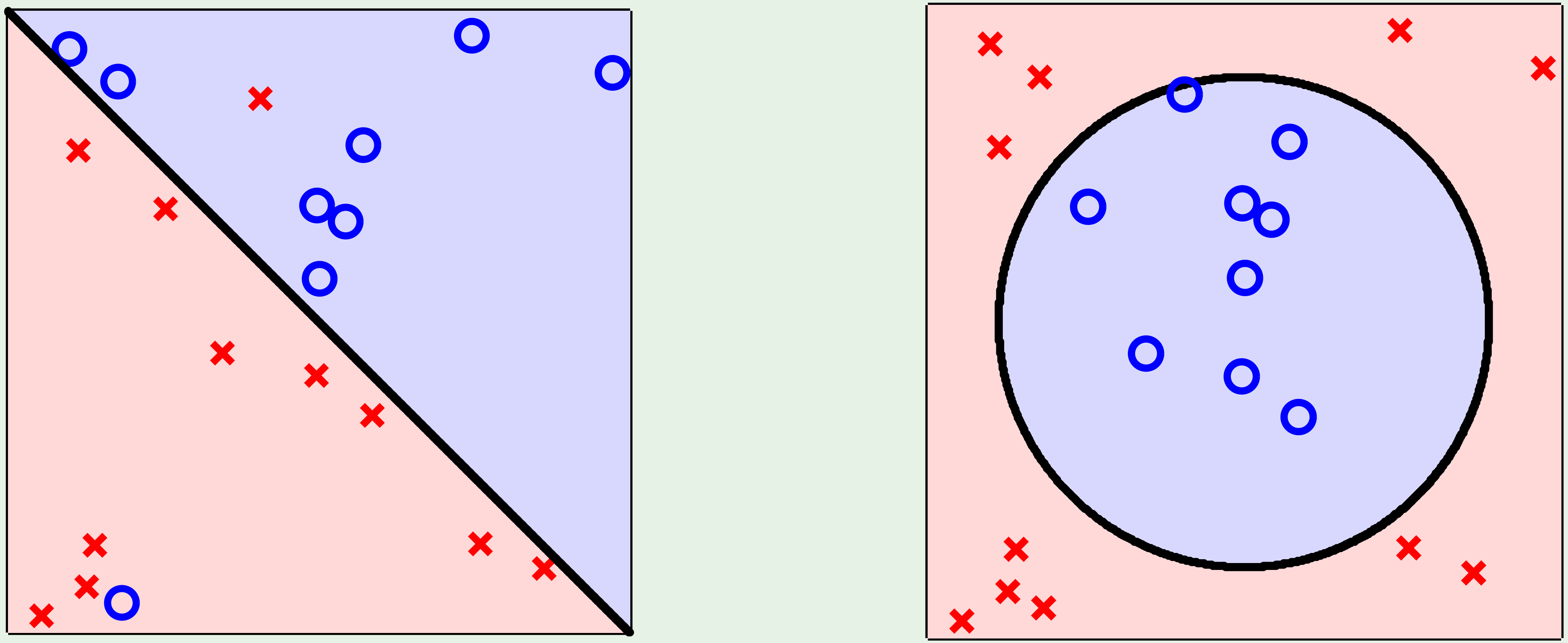
$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \quad \xrightarrow{\Phi} \quad \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots\cdots, z_{\tilde{d}})$$

$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

$$\mathbf{w} \qquad\qquad\qquad\qquad \tilde{\mathbf{w}}$$

$$d_{\mathrm{VC}} = d + 1 \qquad\qquad\qquad d_{\mathrm{VC}} \le \tilde{d} + 1$$

Two non-separable cases

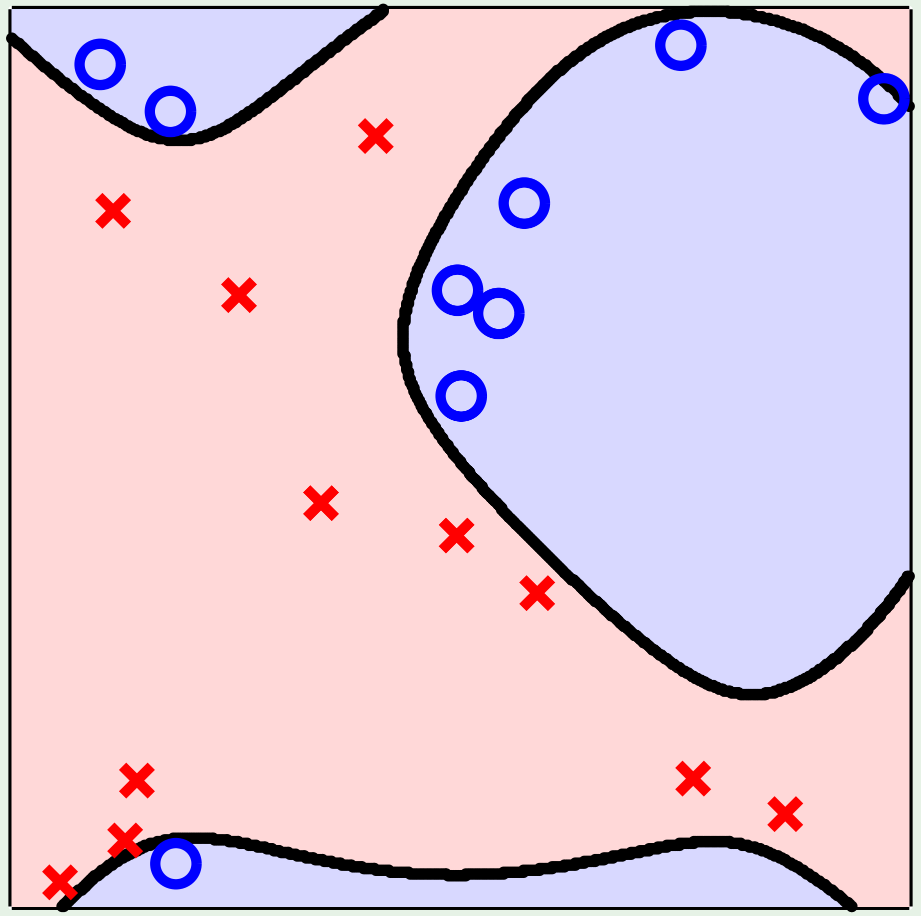


First case

Use a linear model in $\mathcal{X}$; accept $E_{\text{in}} > 0$

or

Insist on $E_{\text{in}} = 0$; go to high-dimensional $\mathcal{Z}$



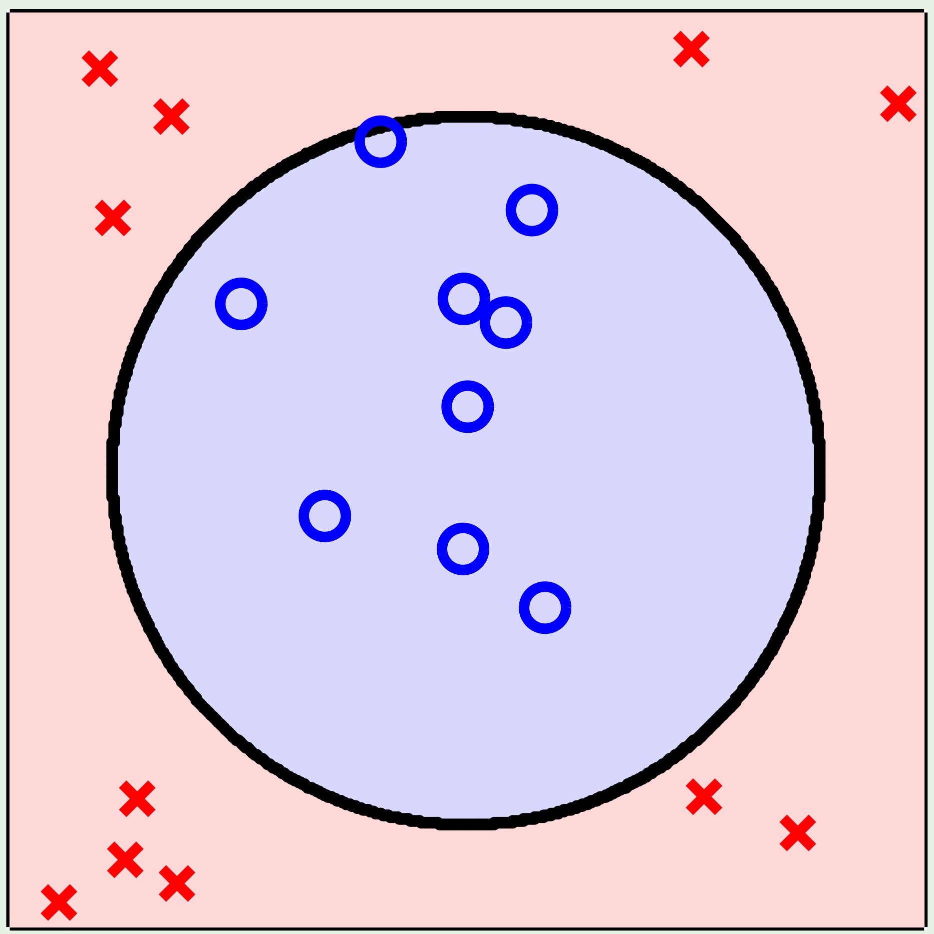
Second case

$\mathbf{z} = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$

Why not: $\mathbf{z} = (1, x_1^2, x_2^2)$

or better yet: $\mathbf{z} = (1, x_1^2 + x_2^2)$

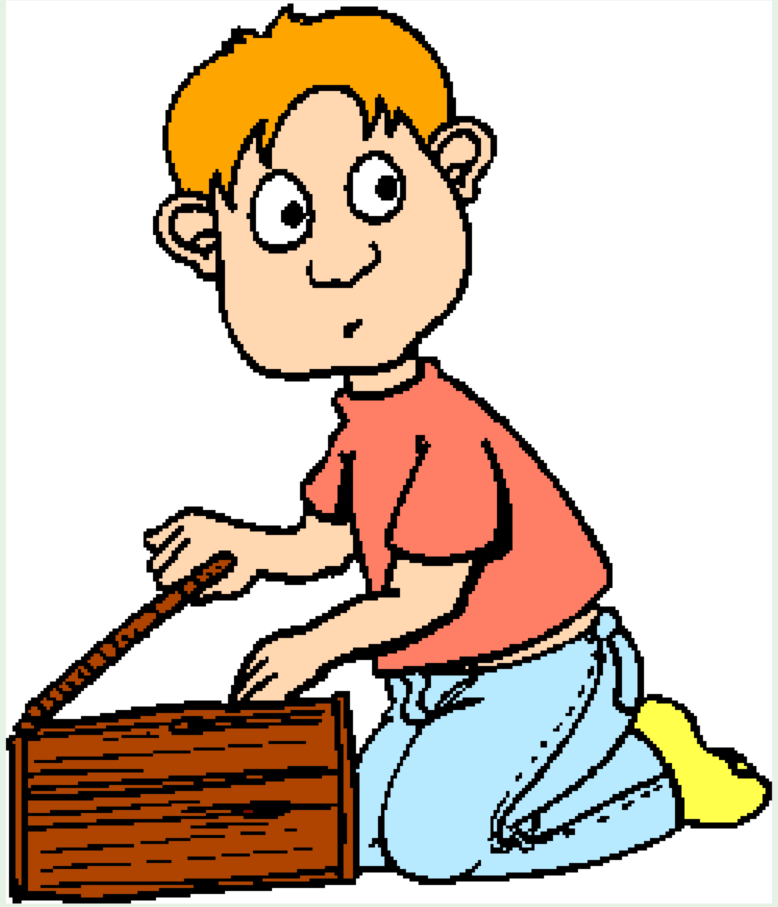
or even: $\mathbf{z} = (x_1^2 + x_2^2 - 0.6)$



Lesson learned

Looking at the data *before* choosing the model can be hazardous to your E_{out}

Data snooping



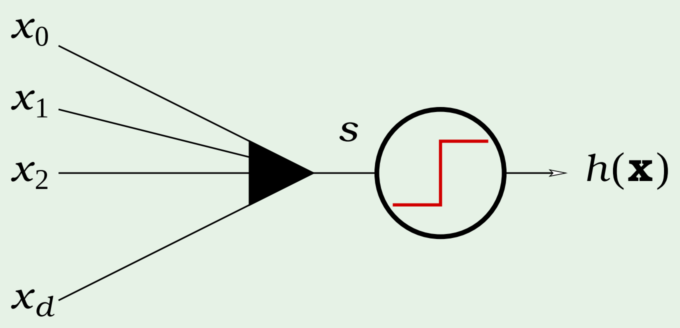
Logistic regression - Outline

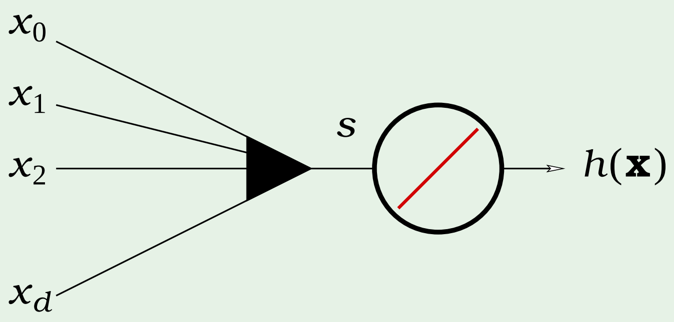
- The model
- Error measure
- Learning algorithm

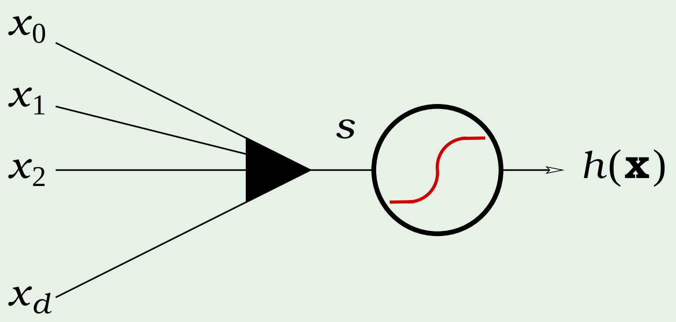
A third linear model

$$s = \sum_{i=0}^{d} w_i x_i$$

linear classification	linear regression	**logistic regression**
$h(\mathbf{x}) = \text{sign}(s)$	$h(\mathbf{x}) = s$	$h(\mathbf{x}) = \theta(s)$



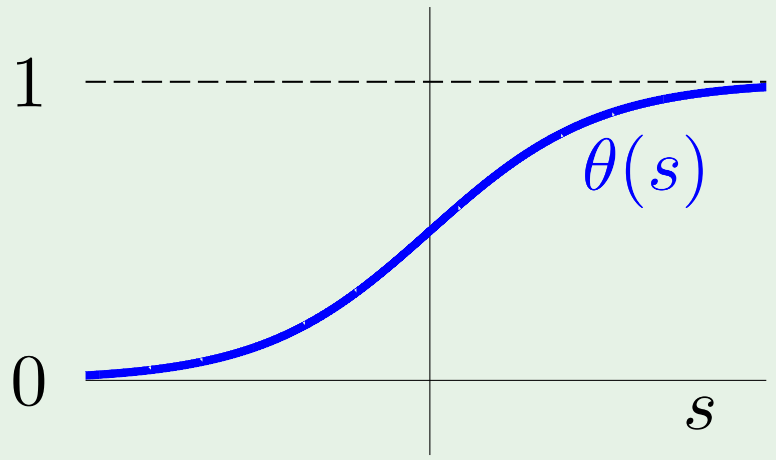




The logistic function θ

The formula:

$$\theta(s) = \frac{e^s}{1 + e^s}$$



soft threshold: uncertainty

sigmoid: flattened out 's'

Probability interpretation

$h(\mathbf{x}) = \theta(s)$ is interpreted as a probability

Example. Prediction of heart attacks

Input $\mathbf{x}$: cholesterol level, age, weight, etc.

$\theta(s)$: probability of a heart attack

The signal $s = \mathbf{w}^{\intercal}\mathbf{x}$ "risk score"

Genuine probability

Data $(\mathbf{x}, y)$ with binary y, generated by a noisy target:

$$P(y \mid \mathbf{x}) \;=\; \begin{cases} f(\mathbf{x}) & \text{for } y = +1; \\ 1 - f(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

The target $f : \mathbb{R}^d \to [0, 1]$ is the probability

Learn $g(\mathbf{x}) \;=\; \theta(\mathbf{w}^{\intercal}\, \mathbf{x}) \;\approx\; f(\mathbf{x})$

Error measure

For each $(\mathbf{x}, y)$, y is generated by probability $f(\mathbf{x})$

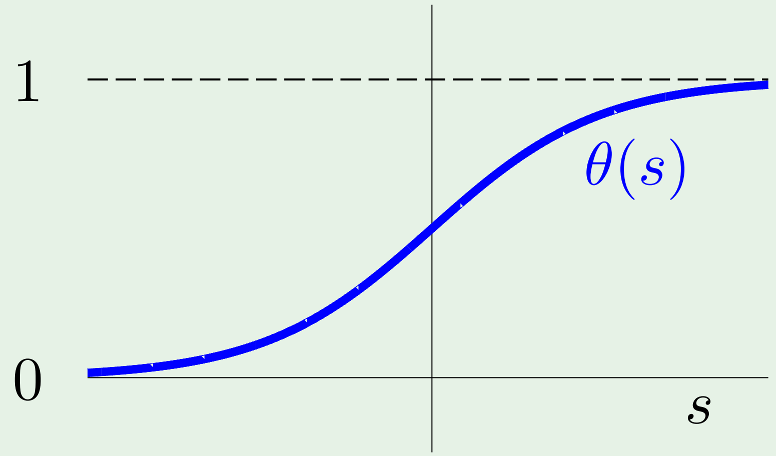
Plausible error measure based on **likelihood:**

If $h = f$, how likely to get y from $\mathbf{x}$?

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

Formula for likelihood

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$



Substitute $h(\mathbf{x}) = \theta(\mathbf{w}^\intercal\mathbf{x})$, noting $\theta(-s) = 1 - \theta(s)$

$$P(y \mid \mathbf{x}) = \theta(y\ \mathbf{w}^\intercal\mathbf{x})$$

Likelihood of $\mathcal{D} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ is

$$\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n\mathbf{w}^\intercal\mathbf{x}_n)$$

Maximizing the likelihood

Minimize $$-\frac{1}{N}\ln\left(\prod_{n=1}^{N}\theta(y_n\,\mathbf{w}^{\mathsf{T}}\,\mathbf{x}_n)\right)$$

$$=\frac{1}{N}\sum_{n=1}^{N}\ln\left(\frac{1}{\theta(y_n\,\mathbf{w}^{\mathsf{T}}\,\mathbf{x}_n)}\right)$$

$$\left[\theta(s)=\frac{1}{1+e^{-s}}\right]$$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\underbrace{\ln\left(1+e^{-y_n\mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right)}_{\mathrm{e}\left(h(\mathbf{x}_n),y_n\right)}$$

"cross-entropy" error

Logistic regression - Outline

- The model

- Error measure

- Learning algorithm

How to minimize E_{in}

For logistic regression,

$$E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\sum_{n=1}^{N} \ln\left(1 + e^{-y_n \mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right) \qquad \longleftarrow \textbf{iterative} \text{ solution}$$

Compare to linear regression:

$$E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - y_n)^2 \qquad \longleftarrow \text{closed-form solution}$$

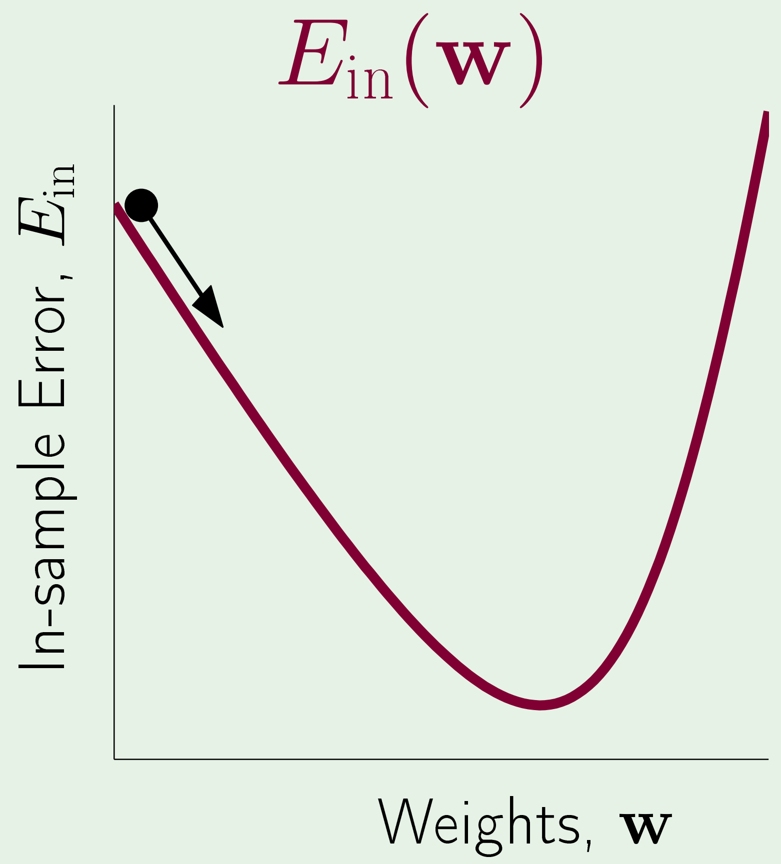
Iterative method: gradient descent

General method for nonlinear optimization

Start at $\mathbf{w}(0)$; take a step along steepest slope

Fixed step size: $\mathbf{w}(1) \;=\; \mathbf{w}(0) + \eta\,\hat{\mathbf{v}}$

What is the direction $\hat{\mathbf{v}}$?



Formula for the direction $\hat{\mathbf{v}}$

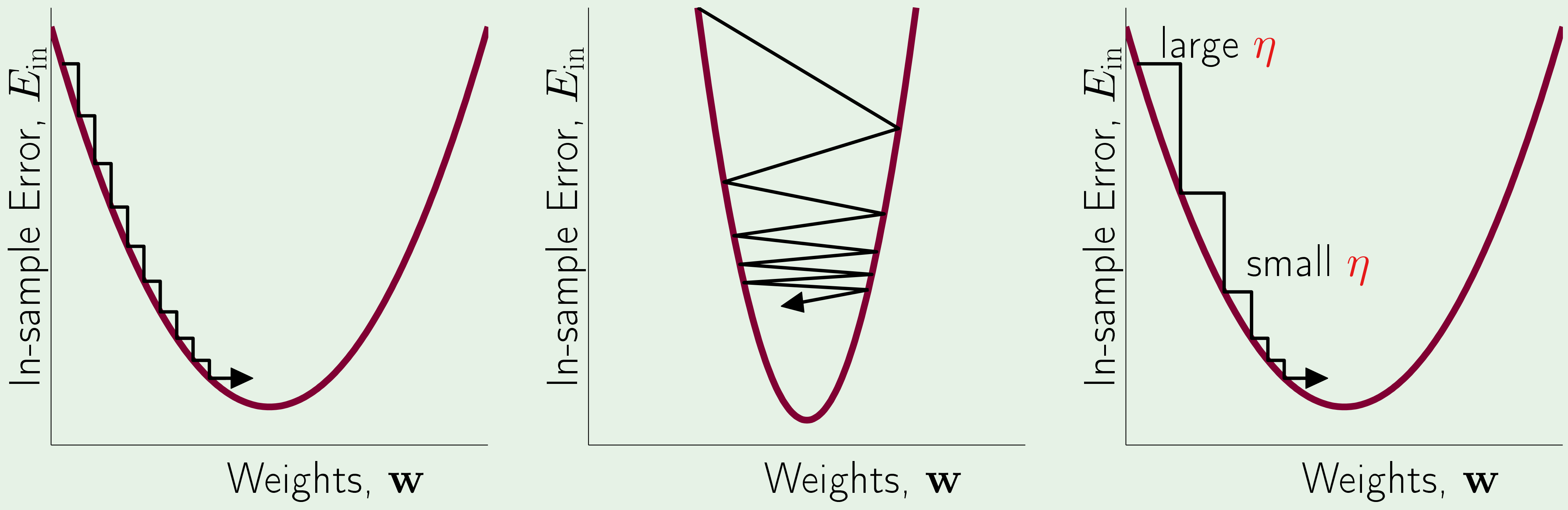
$$\begin{aligned}
\Delta E_{\text{in}} &= E_{\text{in}}(\,\mathbf{w}(0) + \eta\hat{\mathbf{v}}\,) - E_{\text{in}}(\mathbf{w}(0)) \\
&= \eta \nabla E_{\text{in}}(\mathbf{w}(0))^{\mathrm{T}} \hat{\mathbf{v}} + O(\eta^2) \\
&\geq -\eta \|\nabla E_{\text{in}}(\mathbf{w}(0))\|
\end{aligned}$$

Since $\hat{\mathbf{v}}$ is a unit vector,

$$\hat{\mathbf{v}} = -\frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}$$

Fixed-size step?

How η affects the algorithm:



η too small | η too large | variable η – just right

η should increase with the slope

Easy implementation

Instead of

$$\Delta \mathbf{w} = \eta \, \hat{\mathbf{v}}$$

$$= -\eta \frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}$$

Have

$$\Delta \mathbf{w} = -\eta \ \nabla E_{\text{in}}(\mathbf{w}(0))$$

Fixed **learning rate** η

Logistic regression algorithm

Initialize the weights at $t = 0$ to $\mathbf{w}(0)$

for $t = 0, 1, 2, \ldots$ **do**

  Compute the gradient

$$\nabla E_{\text{in}} = -\frac{1}{N}\sum_{n=1}^{N}\frac{y_n \mathbf{x}_n}{1 + e^{y_n \mathbf{w}^{\intercal}(t)\mathbf{x}_n}}$$

  Update the weights: $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E_{\text{in}}$

  Iterate to the next step until it is time to stop

Return the final weights $\mathbf{w}$

Summary of Linear Models