Learning From Data
Lecture 22
Neural Networks and Overfitting

Approximation vs. Generalization
Regularization and Early Stopping
Minimizing E_{in} More Efficienty ☺

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CSCI 4100/6100

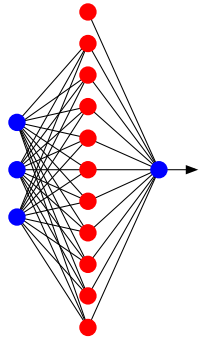
RECAP: Neural Networks and Fitting the Data

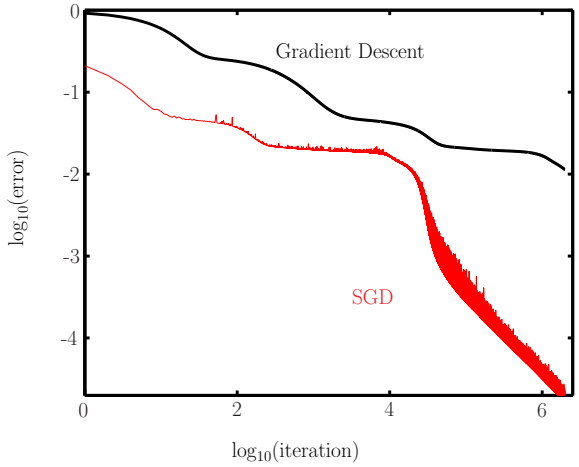
Forward Propagation:

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x})$$

$$\mathbf{s}^{(\ell)} = (\mathrm{W}^{(\ell)})^{\mathrm{T}}\mathbf{x}^{(\ell-1)} \qquad \mathbf{x}^{(\ell)} = \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$$

(Compute h and E_{in})
Choose $\mathrm{W} = \{\mathrm{W}^{(1)}, \mathrm{W}^{(1)}, \ldots, \mathrm{W}^{(L)}\}$ to minimize E_{in}



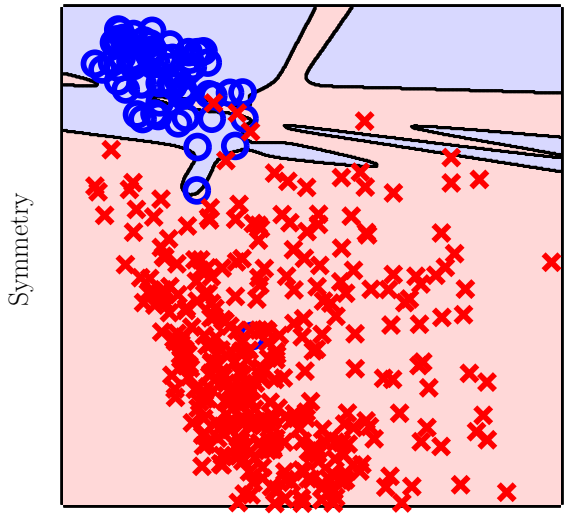


Gradient descent:

$$\mathrm{W}(t+1) \leftarrow \mathrm{W}(t) - \eta \nabla E_{\text{in}}(\mathrm{W}(t))$$

Compute gradient $\longrightarrow$ need $\dfrac{\partial \mathsf{e}}{\partial \mathrm{W}^{(\ell)}} \longrightarrow$ need $\boldsymbol{\delta}^{(\ell)} = \dfrac{\partial \mathsf{e}}{\partial \mathbf{s}^{(\ell)}}$

$$\frac{\partial \mathsf{e}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

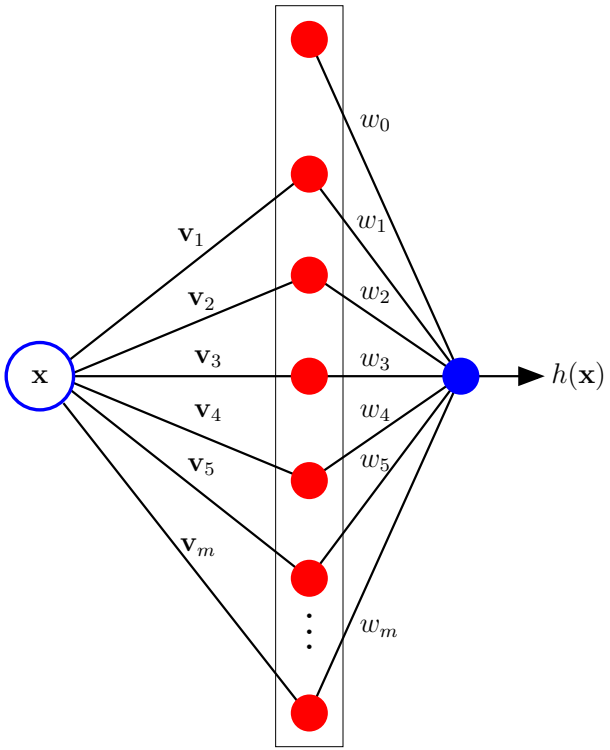


Backpropagation:

$$\boldsymbol{\delta}^{(1)} \longleftarrow \boldsymbol{\delta}^{(2)} \cdots \longleftarrow \boldsymbol{\delta}^{(L-1)} \longleftarrow \boldsymbol{\delta}^{(L)}$$

$$\boldsymbol{\delta}^{(\ell)} = \theta'(\mathbf{s}^{(\ell)}) \otimes \left[\mathrm{W}^{(\ell+1)}\boldsymbol{\delta}^{(\ell+1)}\right]_1^{d^{(\ell)}}$$

2-Layer Neural Network



$$h(\mathbf{x}) = \theta\left(w_0 + \sum_{j=1}^{m} w_j \theta\left(\mathbf{v}_j{}^{\mathrm{T}}\mathbf{x}\right)\right)$$

The Neural Network has a Tunable Transform

Neural Network

$$h(\mathbf{x}) = \theta\left(w_0 + \sum_{j=1}^{m} w_j \theta\left(\mathbf{v}_j{}^{\mathrm{T}}\mathbf{x}\right)\right)$$

Nonlinear Transform

$$h(\mathbf{x}) = \theta\left(w_0 + \sum_{j=1}^{\tilde{d}} w_j \Phi_j(\mathbf{x})\right)$$

k-RBF-Network

$$h(\mathbf{x}) = \theta\left(w_0 + \sum_{j=1}^{k} w_j \phi\left(\|\,\mathbf{x} - \boldsymbol{\mu}_j\,\|\right)\right)$$

$$E_{\text{in}} = O\left(\frac{1}{m}\right)$$

↑
approximation

Generalization

MLP:

$$d_{\text{VC}} = O(md \log(md))$$

$$m = \sqrt{N}$$

(convergence to optimal for MLP, just like k-NN)

semi-parametric because you still have to learn parameters.

tanh :

$$d_{\text{VC}} = O(md(m + d))$$

Regularization – Weight Decay

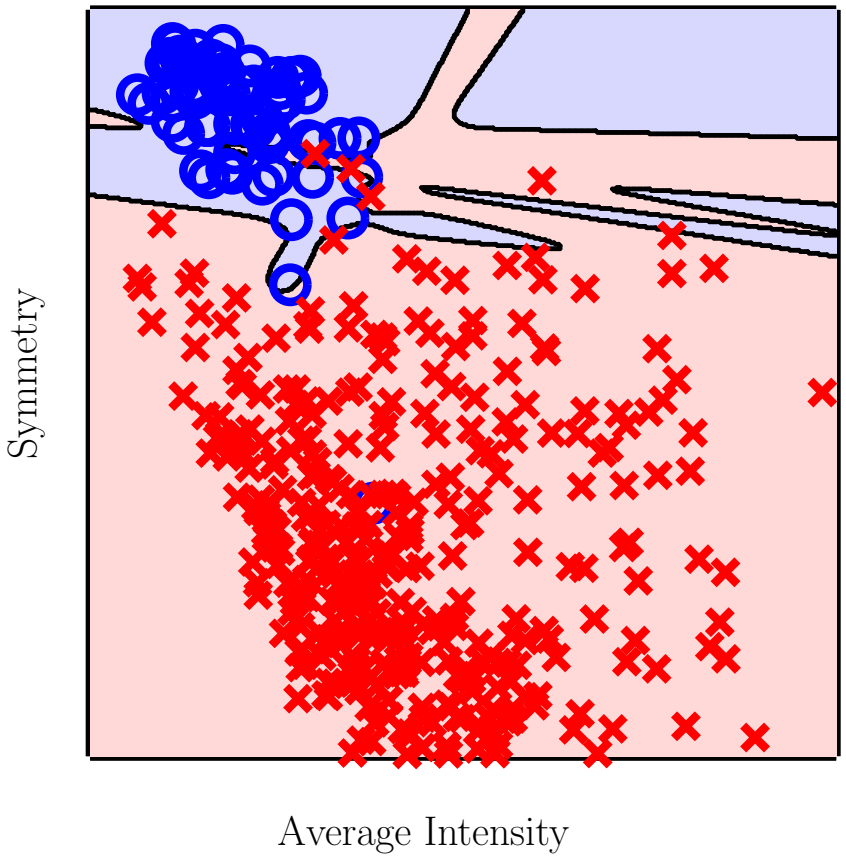
$$E_{\text{aug}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(h(\mathbf{x}_n;\mathbf{w}) - y_n)^2 + \frac{\lambda}{N}\sum_{\ell,i,j}(w_{ij}^{(\ell)})^2$$

$$\frac{\partial E_{\text{aug}}(\mathbf{w})}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial \mathrm{W}^{(\ell)}} + \frac{2\lambda}{N}\mathrm{W}^{(\ell)}$$

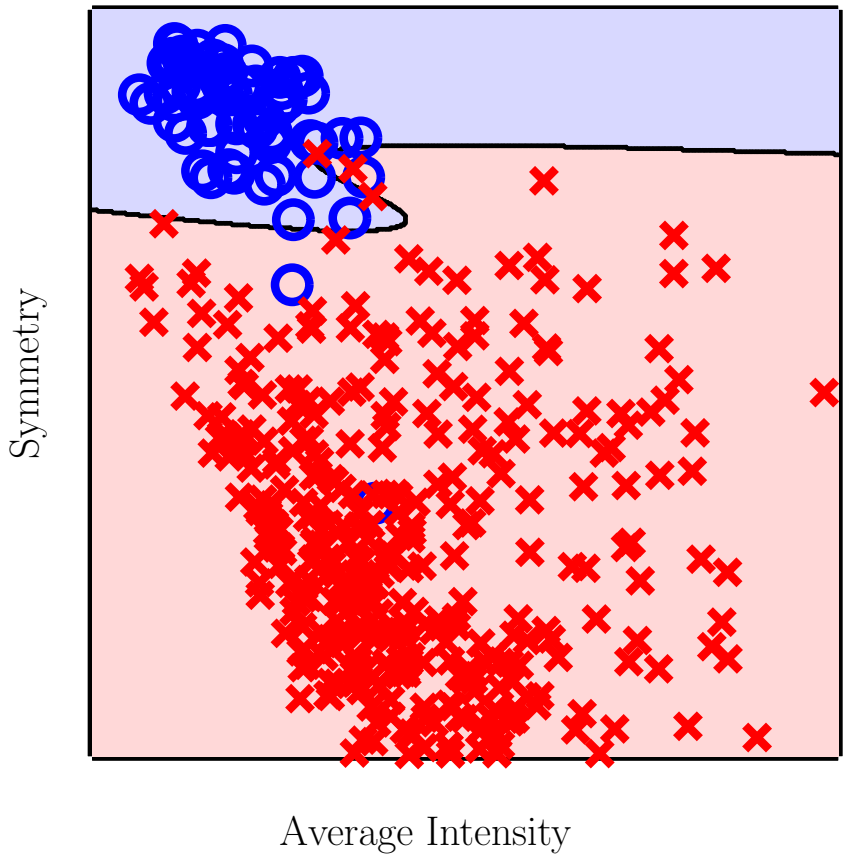
↑
backpropagation

Weight Decay with Digits Data

No Weight Decay

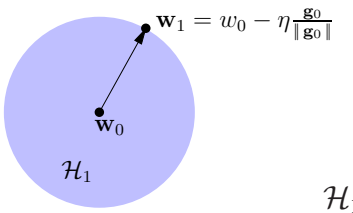


Weight Decay, $\lambda = 0.01$

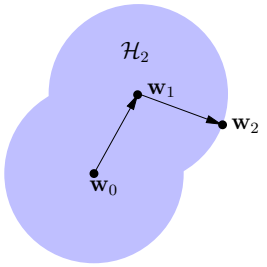


Early Stopping

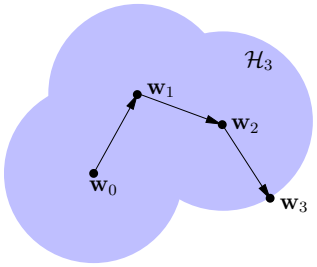
Gradient Descent



$$\mathcal{H}_1 = \{\mathbf{w} : \|\mathbf{w} - \mathbf{w}_0\| \leq \eta\}$$



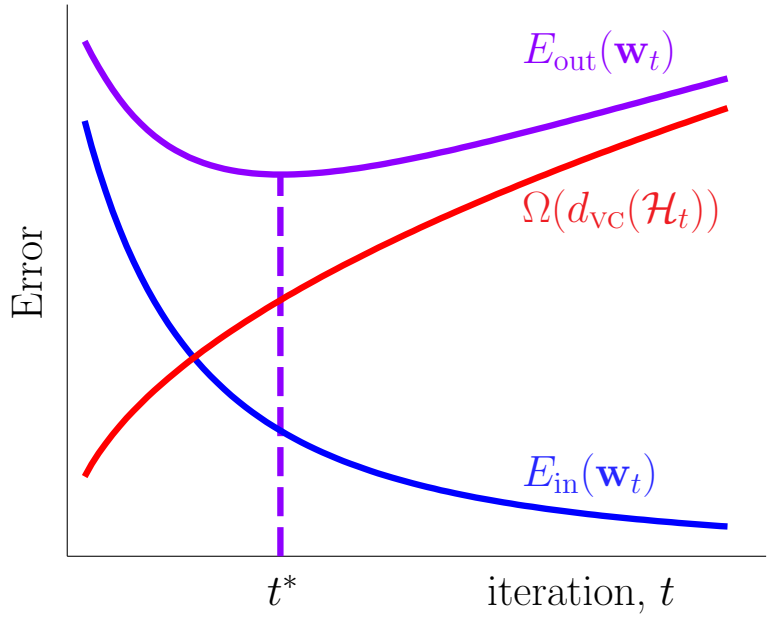
$$\mathcal{H}_2 = \mathcal{H}_1 \cup \{\mathbf{w} : \|\mathbf{w} - \mathbf{w}_1\| \leq \eta\}$$

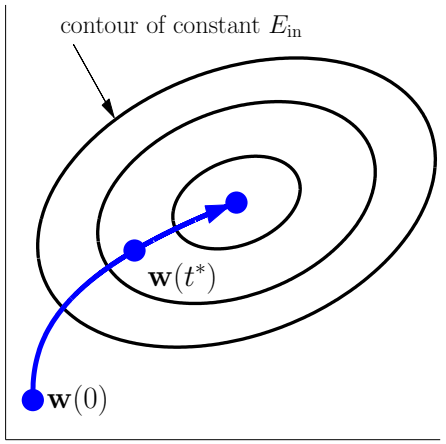


$$\mathcal{H}_3 = \mathcal{H}_2 \cup \{\mathbf{w} : \|\mathbf{w} - \mathbf{w}_2\| \leq \eta\}$$

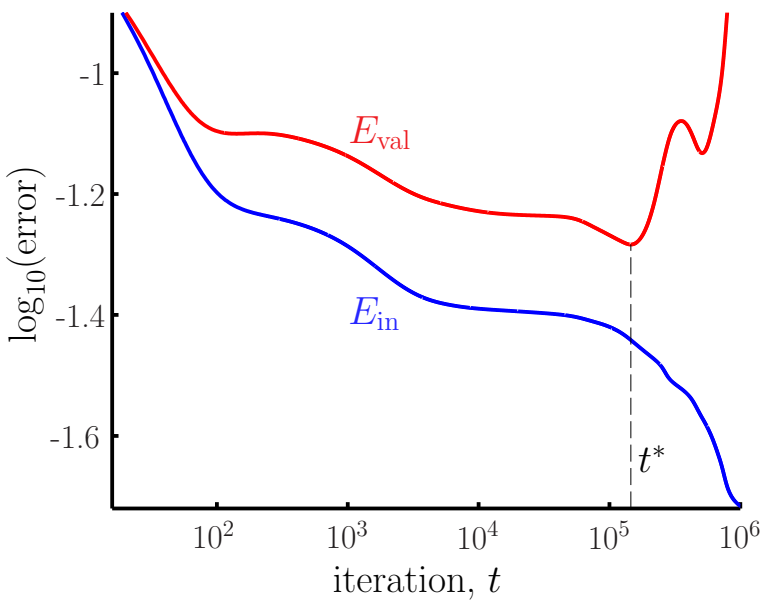
Each iteration explores a larger $\mathcal{H}$

$$\mathcal{H}_1 \subset \mathcal{H}_2 \subset \mathcal{H}_3 \subset \mathcal{H}_4 \subset \cdots$$

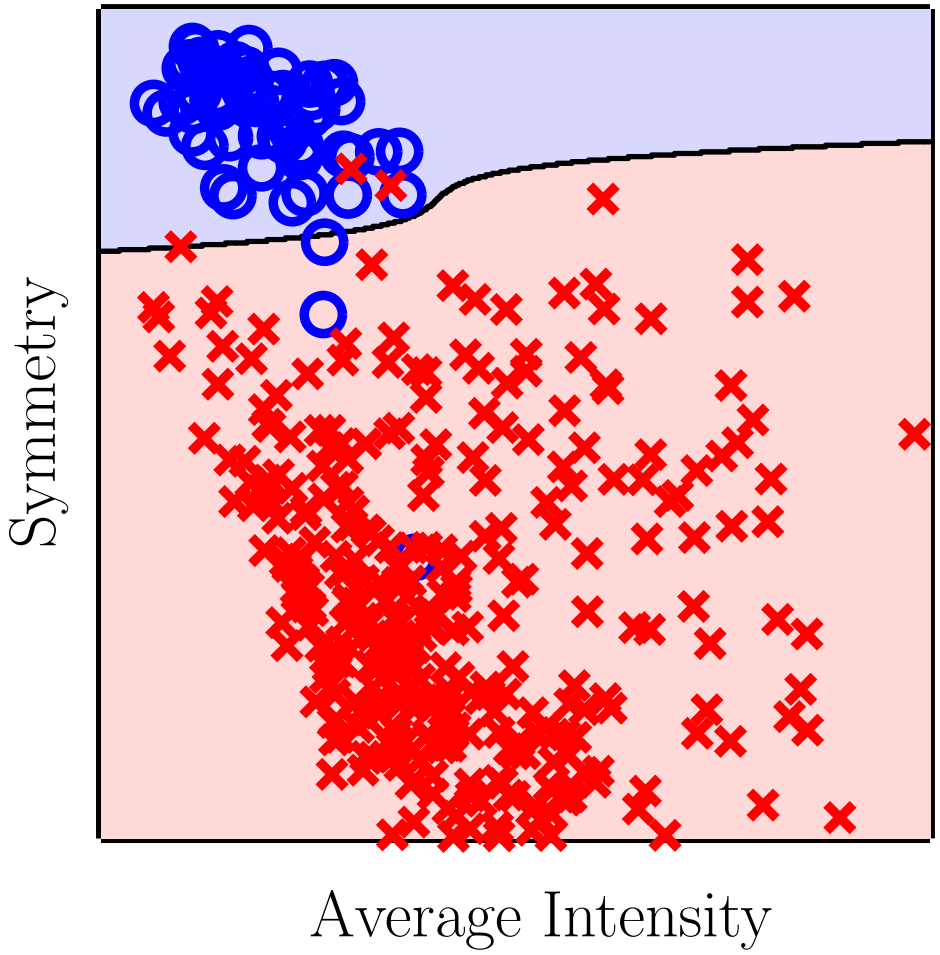




Early Stopping on Digits Data

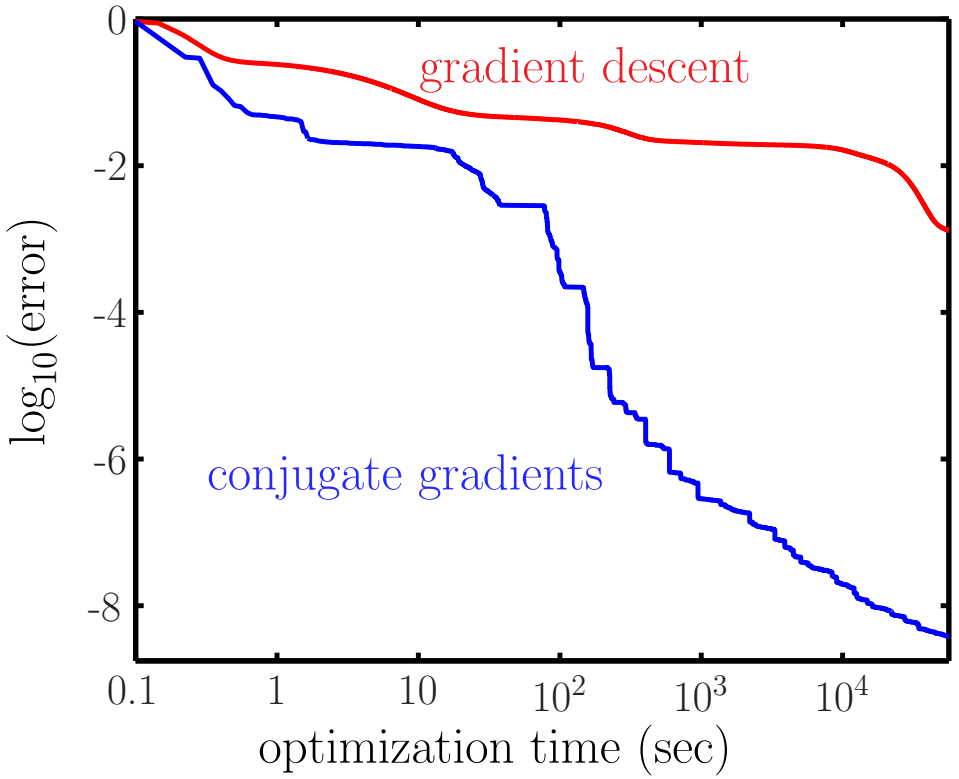


Use a validation set to determine t^*
Output $\mathbf{w}^*$, do not retrain with all the data till t^*.



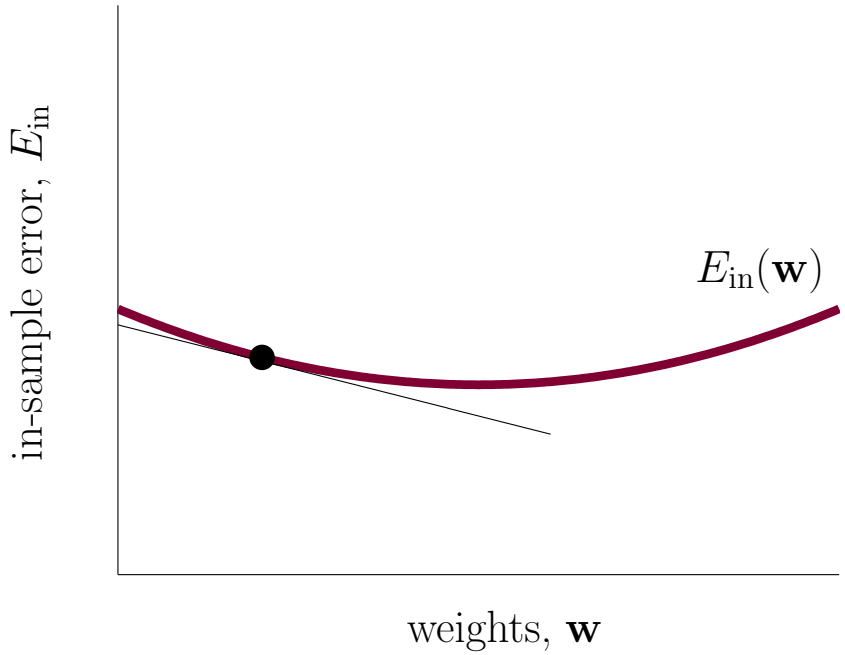
Minimizing E_{in}

1. Use regression for classification
2. Use better algorithms than gradient descent

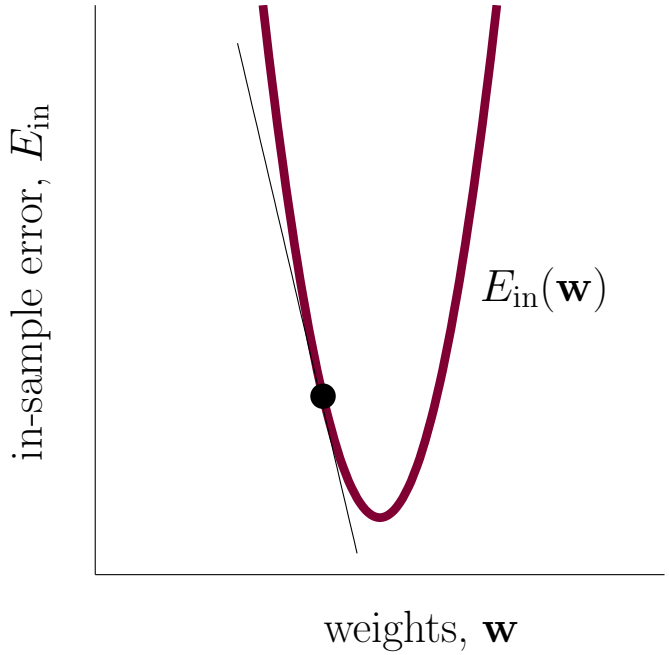


Beefing Up Gradient Descent

Determine the gradient $\mathbf{g}$



Shallow: use large η.



Deep: use small η.

Variable Learning Rate Gradient Descent

1: Initialize $\mathbf{w}(0)$, and η_0 at $t = 0$. Set $\alpha > 1$ and $\beta < 1$.

2: **while** stopping criterion has not been met **do**

3: Let $\mathbf{g}(t) = \nabla E_{\text{in}}(\mathbf{w}(t))$, and set $\mathbf{v}(t) = -\mathbf{g}(t)$.

4: **if** $E_{\text{in}}(\mathbf{w}(t) + \eta_t \mathbf{v}(t)) < E_{\text{in}}(\mathbf{w}(t))$ **then**

5: accept: $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta_t \mathbf{v}(t)$;
increment η: $\eta_{t+1} = \alpha \eta_t$. $\alpha \in [1.05, 1.1]$

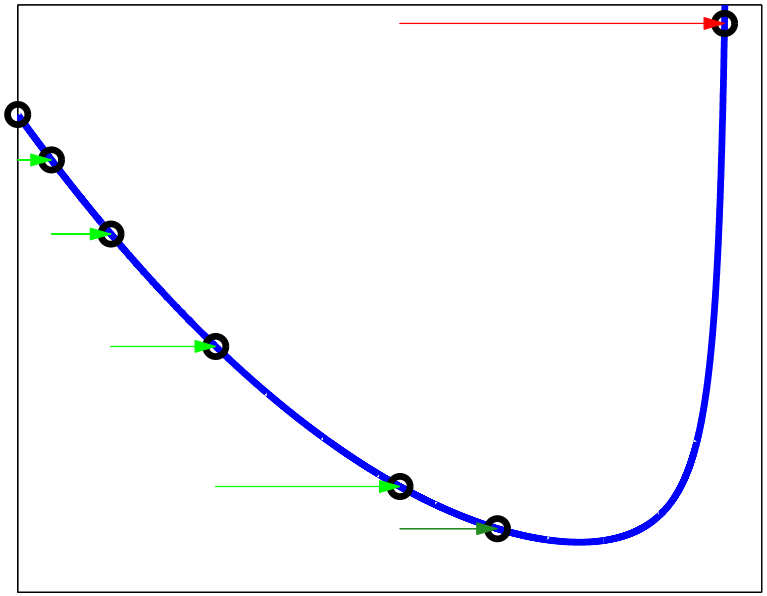
6: **else**

7: reject: $\mathbf{w}(t+1) = \mathbf{w}(t)$;
decrease η: $\eta_{t+1} = \beta \eta_t$. $\beta \in [0.7, 0.8]$

8: **end if**

9: Iterate to the next step, $t \leftarrow t + 1$.

10: **end while**



Steepest Descent - Line Search

1: Initialize $w(0)$ and set $t = 0$;

2: **while** stopping criterion has not been met **do**

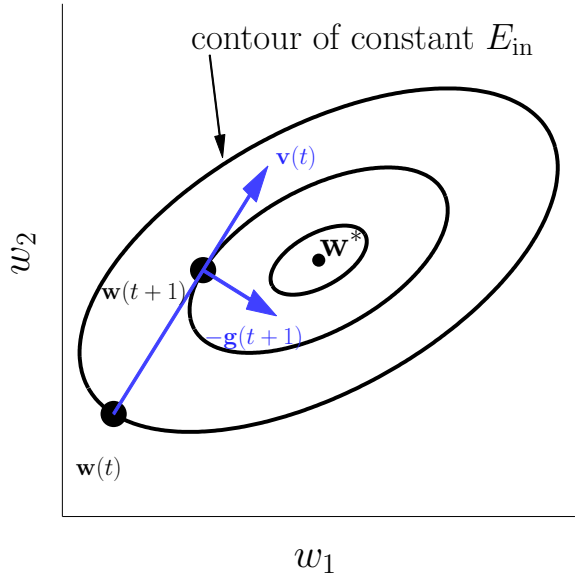
3: Let $\mathbf{g}(t) = \nabla E_{\text{in}}(\mathbf{w}(t))$, and set $\mathbf{v}(t) = -\mathbf{g}(t)$.

4: Let $\eta^* = \text{argmin}_\eta \, E_{\text{in}}(\mathbf{w}(t) + \eta \mathbf{v}(t))$.

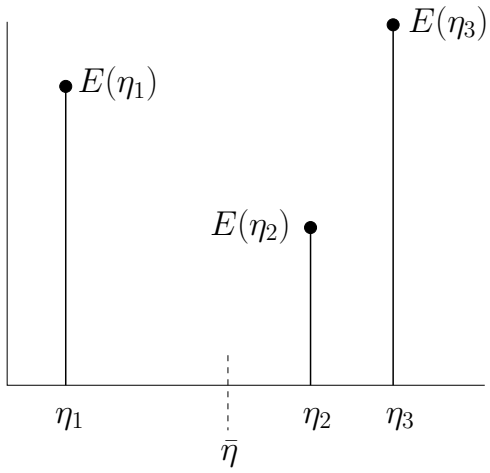
5: $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta^* \mathbf{v}(t)$.

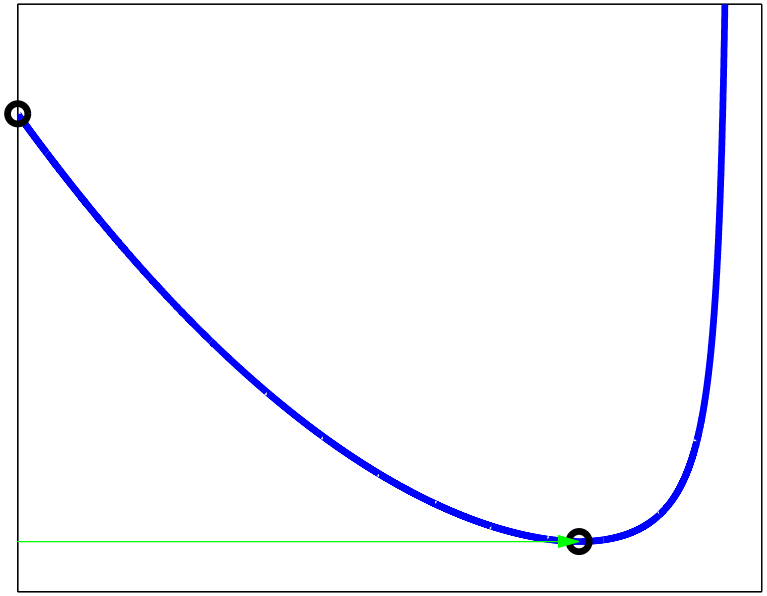
6: Iterate to the next step, $t \leftarrow t + 1$.

7: **end while**

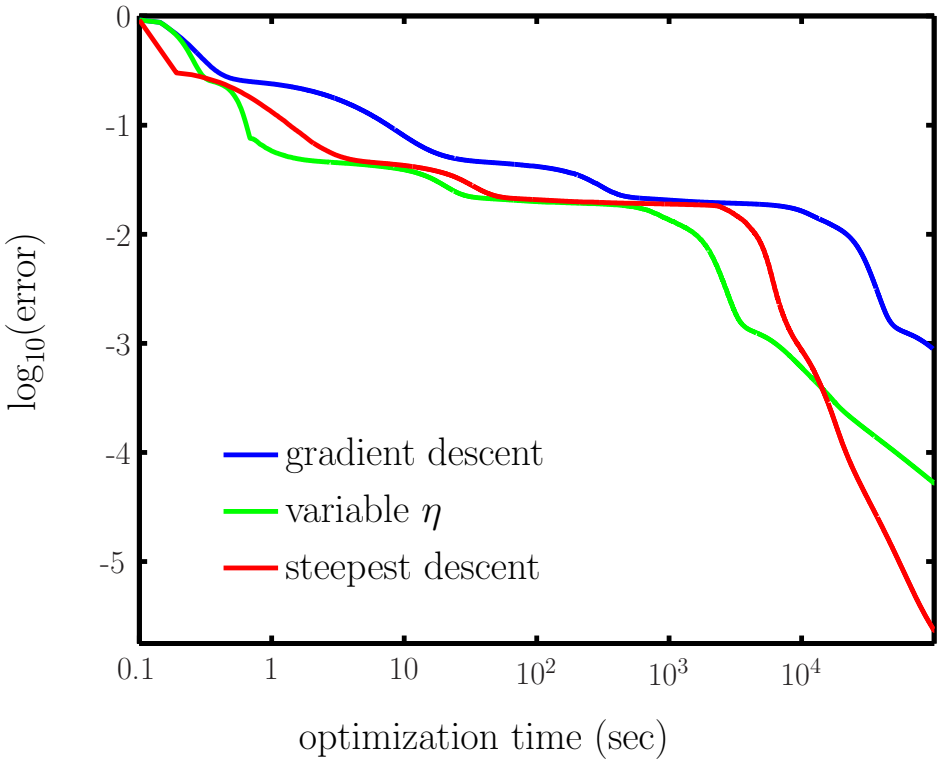


How to accomplish the line search (step 4)?
Simple bisection (binary search) suffices in practice





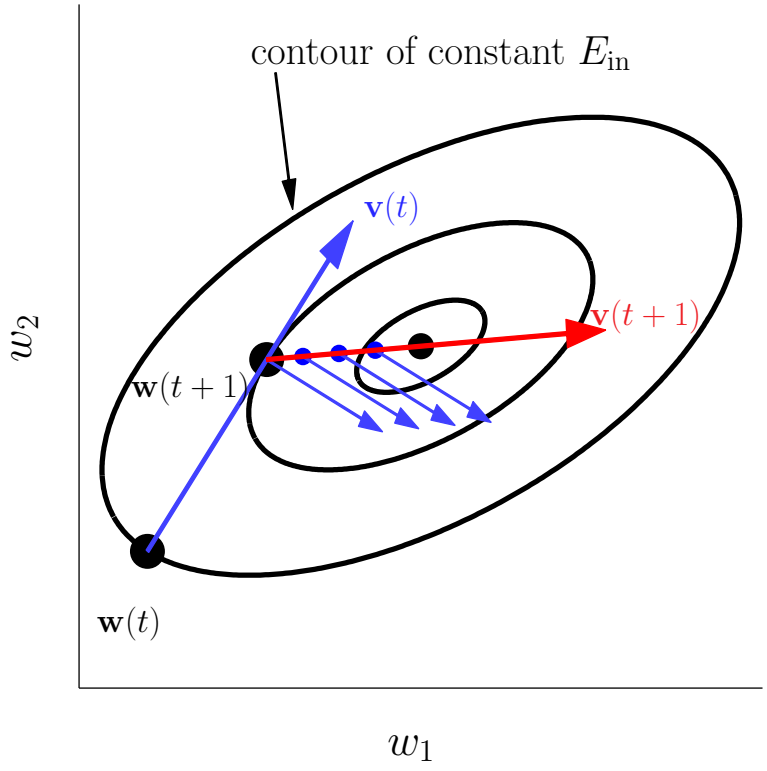
Comparison of Optimization Heuristics

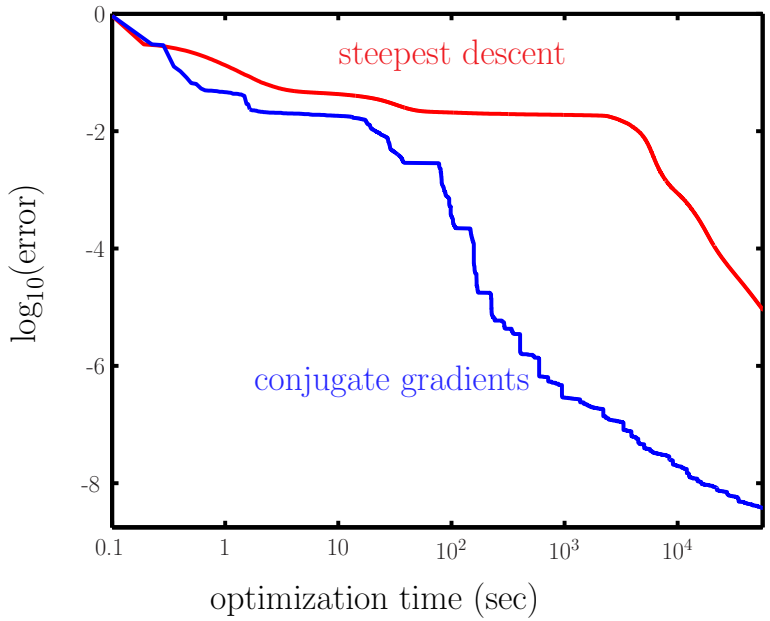


Method	Optimization Time		
	10 sec	1,000 sec	50,000 sec
Gradient Descent	0.122	0.0214	0.0113
Stochastic Gradient Descent	**0.0203**	**0.000447**	**1.6310×10^{-5}**
Variable Learning Rate	0.0432	0.0180	0.000197
Steepest Descent	0.0497	0.0194	0.000140

Conjugate Gradients

1. Line search just like steepest descent.
2. Choose a better direction than $-\mathbf{g}$





Method	Optimization Time 10 sec	1,000 sec	50,000 sec
Stochastic Gradient Descent	0.0203	0.000447	1.6310×10^{-5}
Steepest Descent	0.0497	0.0194	0.000140
Conjugate Gradients	**0.0200**	$\mathbf{1.13 \times 10^{-6}}$	$\mathbf{2.73 \times 10^{-9}}$

There are better algorithms (eg. Levenberg-Marquardt), but we will stop here ☹