Machine Learning
ITCS 6156/8156

Gradient Descent

Razvan C. Bunescu

Department of Computer Science @ CCI

razvan.bunescu@uncc.edu

ML is Optimization

- Try to find the value for w that minimizes:

$$J(w) = \frac{1}{2}w^2 - 4w + 9$$

$$J(w) = \frac{1}{2}(w - 4)^2 + 1$$

- Set $\nabla J(w) = 0$

  $\Rightarrow w - 4 = 0$

  $\Rightarrow w = 4$

Machine Learning is Optimization

- Parametric ML involves minimizing an **objective function** $J(\mathbf{w})$:
  - Also called **cost function** or **error function**.
  - Want to find $\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} J(\mathbf{w})$

- Numerical optimization procedure:
  1. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
  2. Update $\mathbf{w}^\tau$ to $\mathbf{w}^{\tau+1}$ such that $J(\mathbf{w}^{\tau+1}) \leq J(\mathbf{w}^\tau)$.
  3. Increment $\tau = \tau + 1$.
  4. Repeat from 2 until J cannot be improved anymore.

Gradient-based Optimization

- How to update $\mathbf{w}^{\tau}$ to $\mathbf{w}^{\tau+1}$ such that $J(\mathbf{w}^{\tau+1}) \leq J(\mathbf{w}^{\tau})$?

- Move **w** in the direction of **steepest descent**:

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} + \eta\boldsymbol{\Delta}$$

  - $\boldsymbol{\Delta}$ is the direction of steepest descent, i.e. direction along which J decreases the most.
  - η is the learning rate and controls the magnitude of the change.

Gradient-based Optimization

- Move $\mathbf{w}$ in the direction of **steepest descent**:

  $$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} + \eta\boldsymbol{\Delta}$$

- What is the direction of steepest descent of $J(\mathbf{w})$ at $\mathbf{w}^{\tau}$?
  - The gradient $\nabla J(\mathbf{w})$ is in the direction of steepest ascent.
  - Set $\boldsymbol{\Delta} = -\nabla J(\mathbf{w})$ => the **gradient descent** update:

  $$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta\nabla J(\mathbf{w}^{\tau})$$

Gradient Descent Algorithm

- Want to minimize a function $J : R^{n} \rightarrow R$.
  - J is differentiable and convex.
  - compute gradient of J i.e. *direction of steepest increase*:

$$\nabla J(\mathbf{w}) = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_n}\right]$$

1. Set learning rate $\eta = 0.001$ (or other small value).
2. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
3. Repeat for epochs E or until J does not improve:
4. $\quad \tau = \tau + 1$.
5. $\quad \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$

What if objective is not differentiable?

- **Subgradient methods.**
  - Minimize convex functions that are not necessarily differentiable.
- **Gradient free methods**:
  - **Evolutionary Programming**.
  - **Bayesian Optimization.**
    - https://arxiv.org/abs/1807.02811
  - **Particle swarm optimization.**
  - **Surrogate optimization**
  - **Simmulated annealing.**
  - …

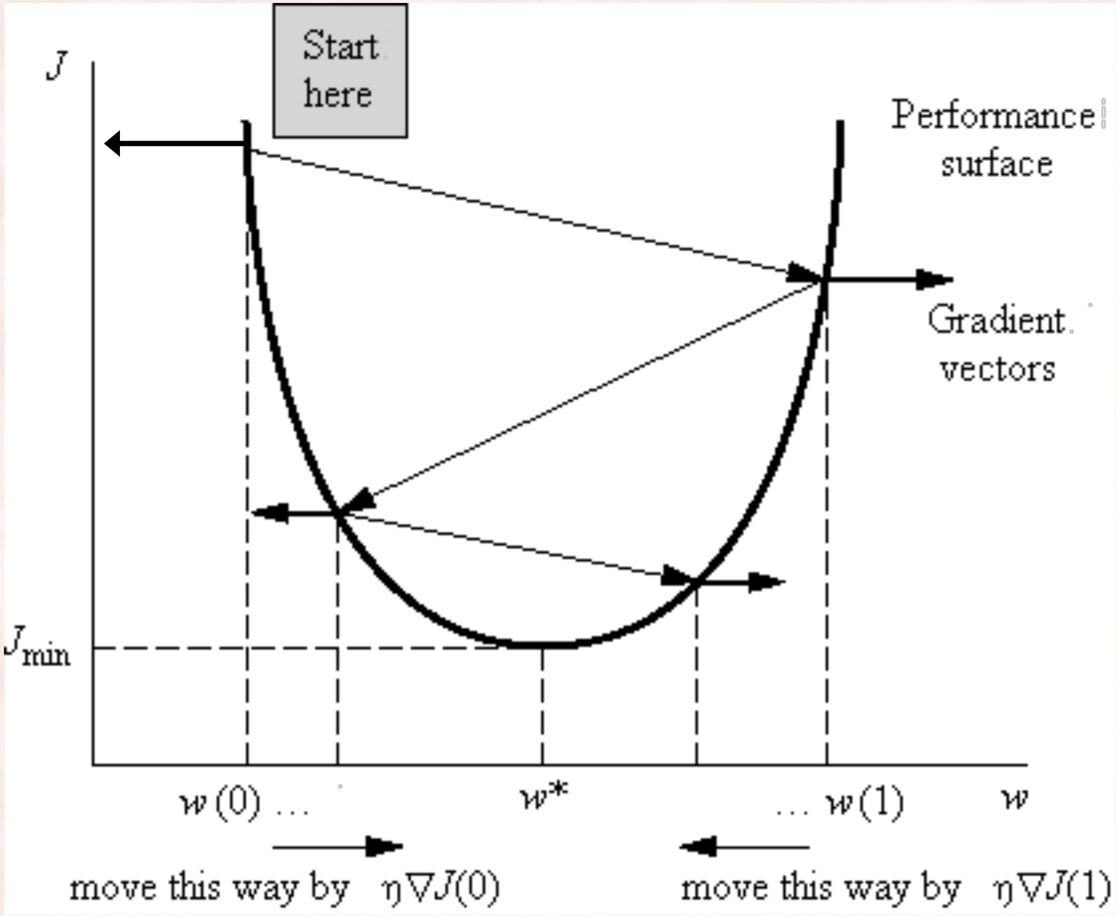
Gradient Descent Algorithm

- Want to minimize a function $J : R^{n} \rightarrow R$.
  - J is differentiable and convex.
  - compute gradient of J i.e. *direction of steepest increase*:

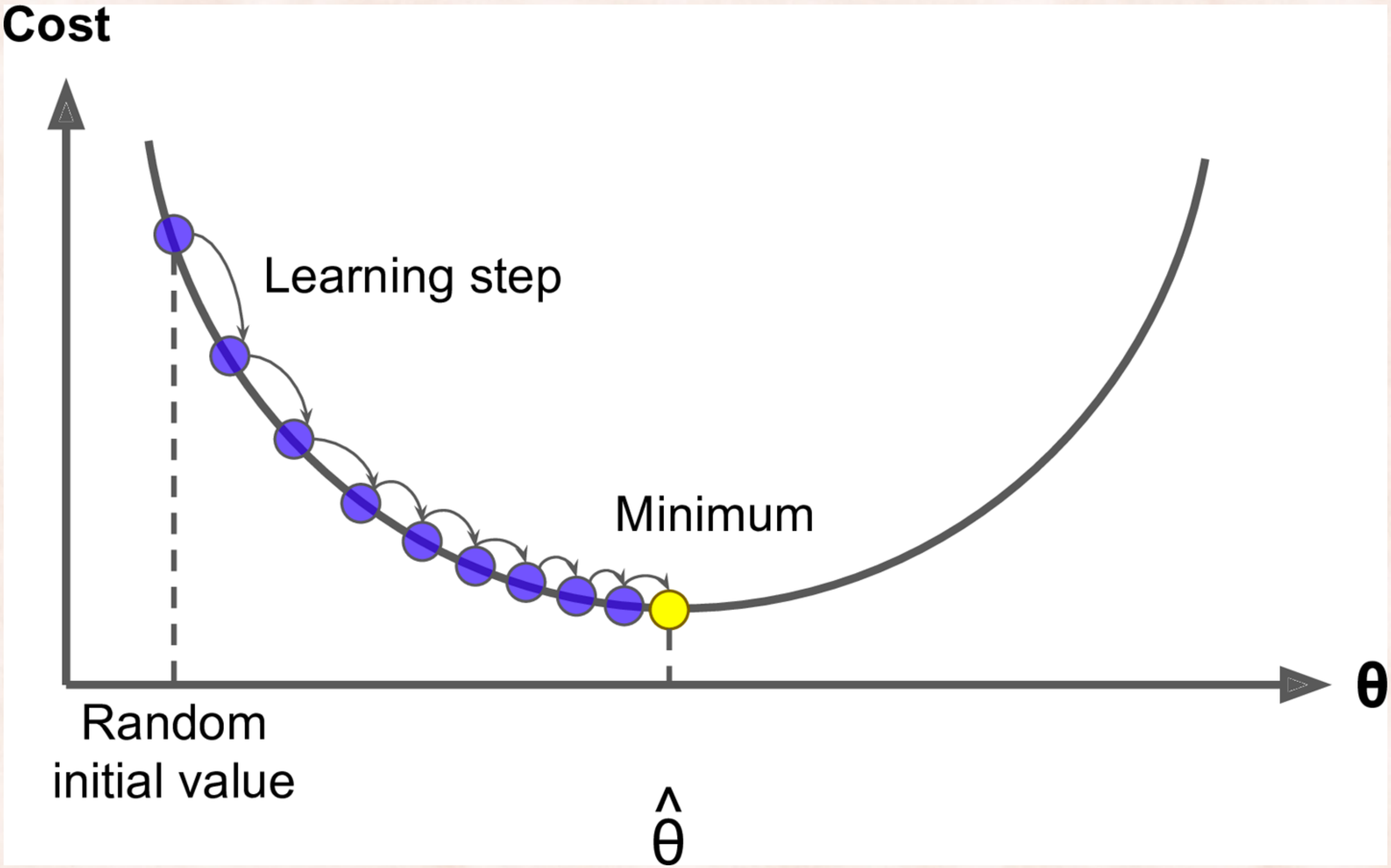
$$\nabla J(\mathbf{w}) = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_n}\right]$$

1. Set learning rate $\eta = 0.001$ (or other small value).
2. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
3. Repeat for epochs E or until J does not improve:
4. $\quad \tau = \tau + 1$.
5. $\quad \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$

Gradient Descent: Large Updates



Gradient Descent: Small Updates



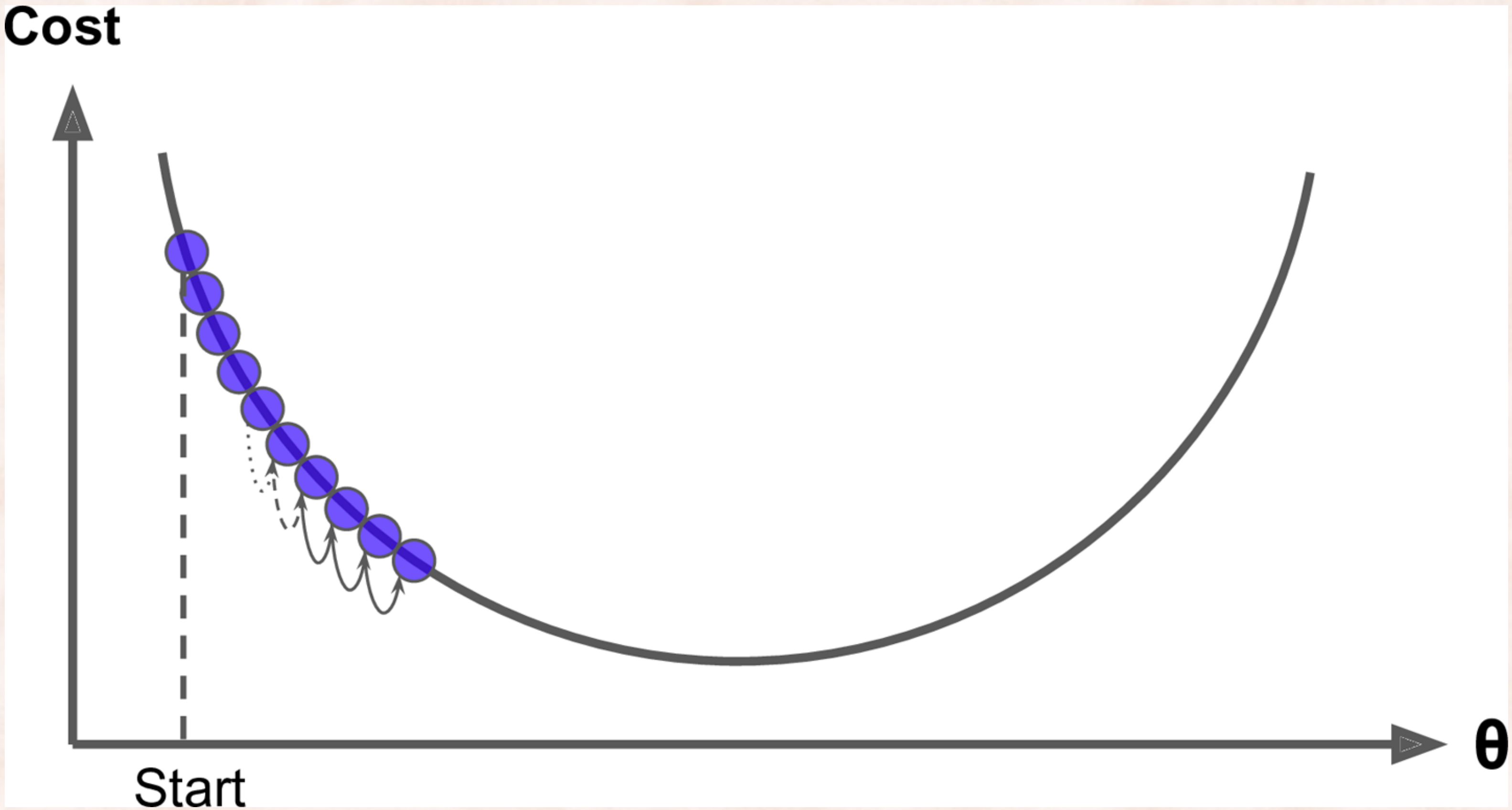
https://www.safaribooksonline.com/library/view/hands-on-machine-learning

The Learning Rate

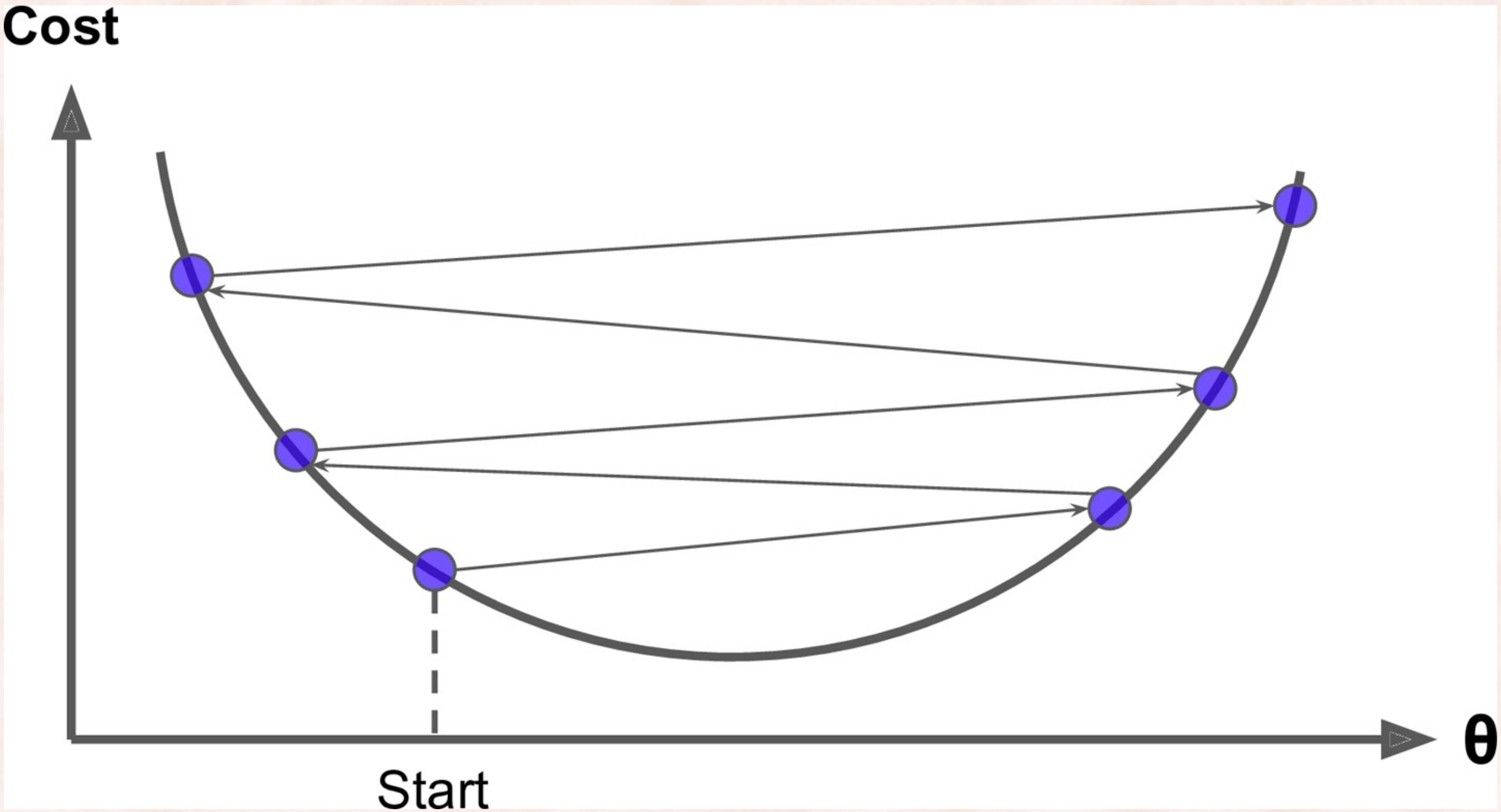
1. Set **learning rate** $\eta = 0.001$ (or other small value).
2. Start with some guess for $\mathbf{w}^0$, set $\tau = 0$.
3. Repeat for epochs E or until J does not improve:
4. $\tau = \tau + 1$.
5. $\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$

- How big should the **learning rate** be?
  - If learning rate too small => slow convergence.
  - If learning rate too big => oscillating behavior => may not even converge.

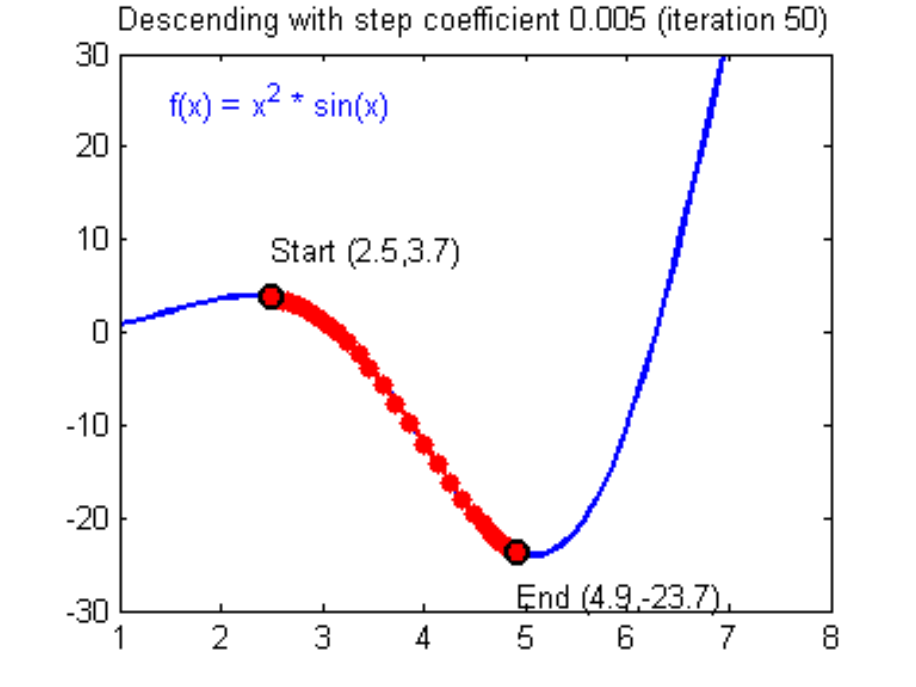
Learning Rate too Small

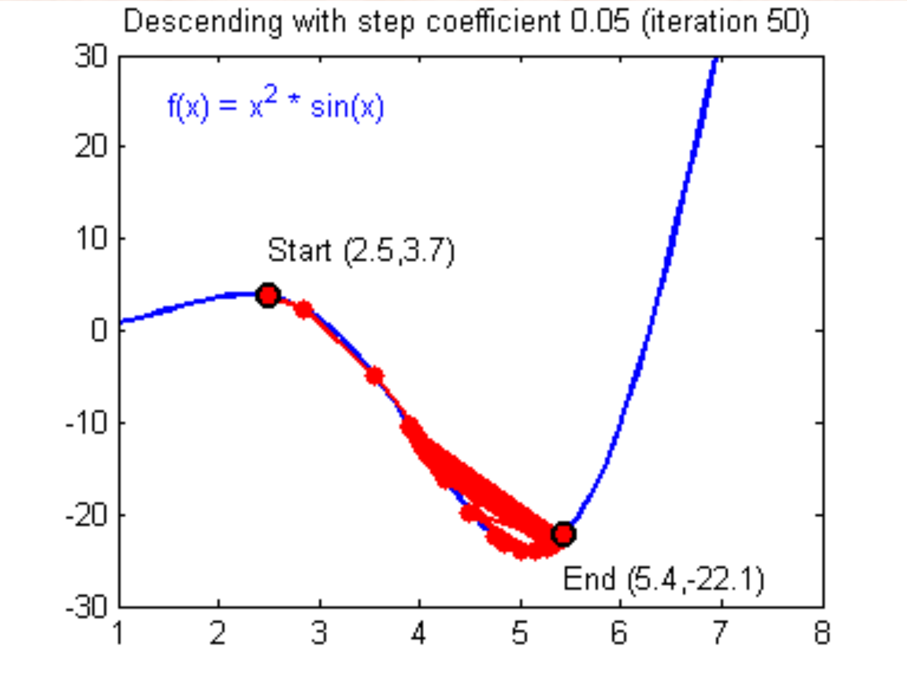


Learning Rate too Large



Learning Rates vs. GD Behavior





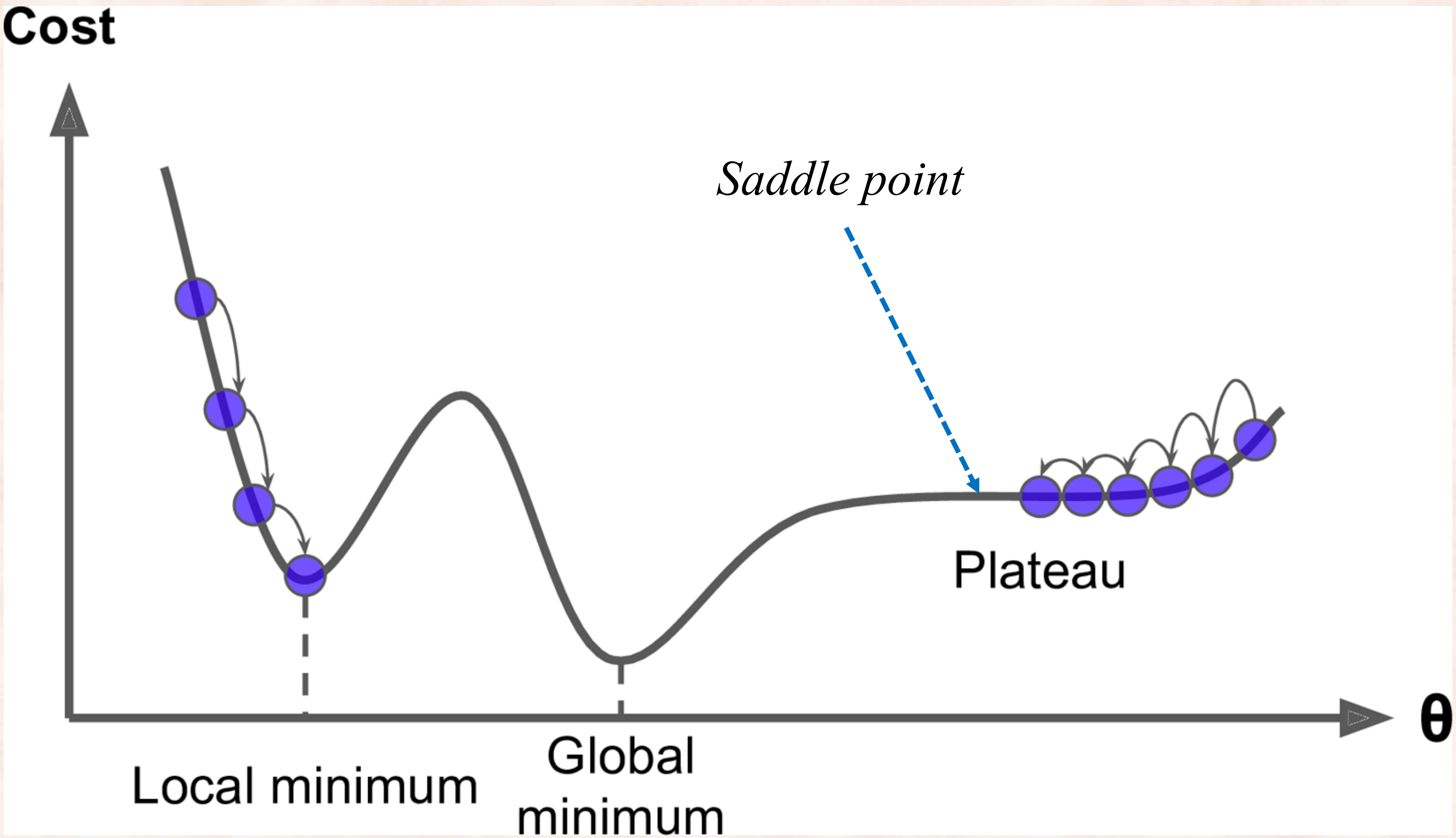
http://scs.ryerson.ca/~aharley/neural-networks/

The Learning Rate

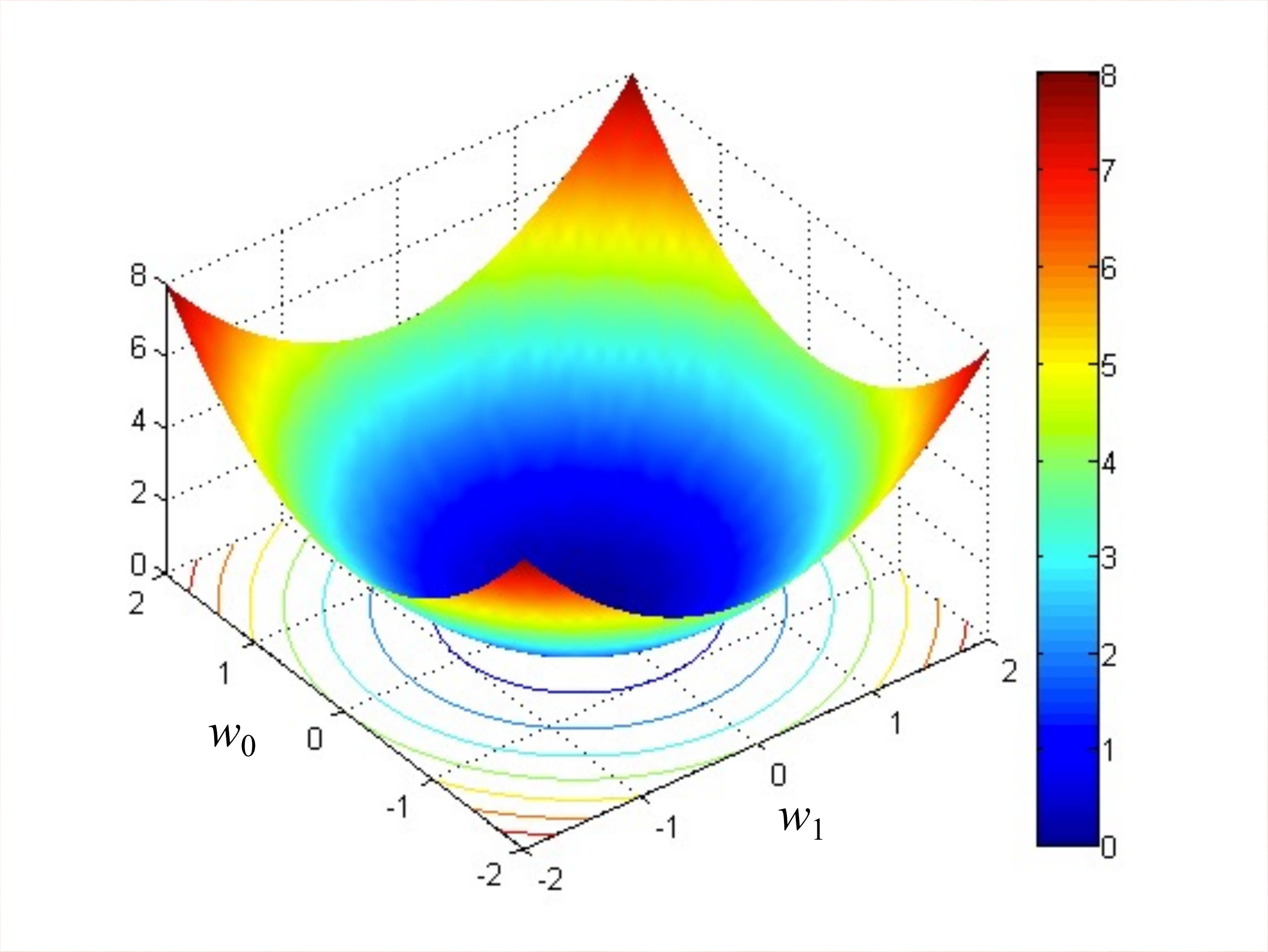
- How big should the **learning rate** be?
  - If learning rate too big => oscillating behavior.
  - If learning rate too small => hinders convergence.

- Use **line search** (backtracking line search, conjugate gradient, …).
- Use **second order methods** (Newton's method, L-BFGS, ...).
  - Requires computing or estimating the Hessian.
- Use a simple learning rate **annealing schedule**:
  - Start with a relatively large value for the learning rate.
  - Decrease the learning rate as a function of the number of epochs or as a function of the improvement in the objective.
- Use **adaptive learning rates**:
  - Adagrad, Adadelta, RMSProp, Adam.

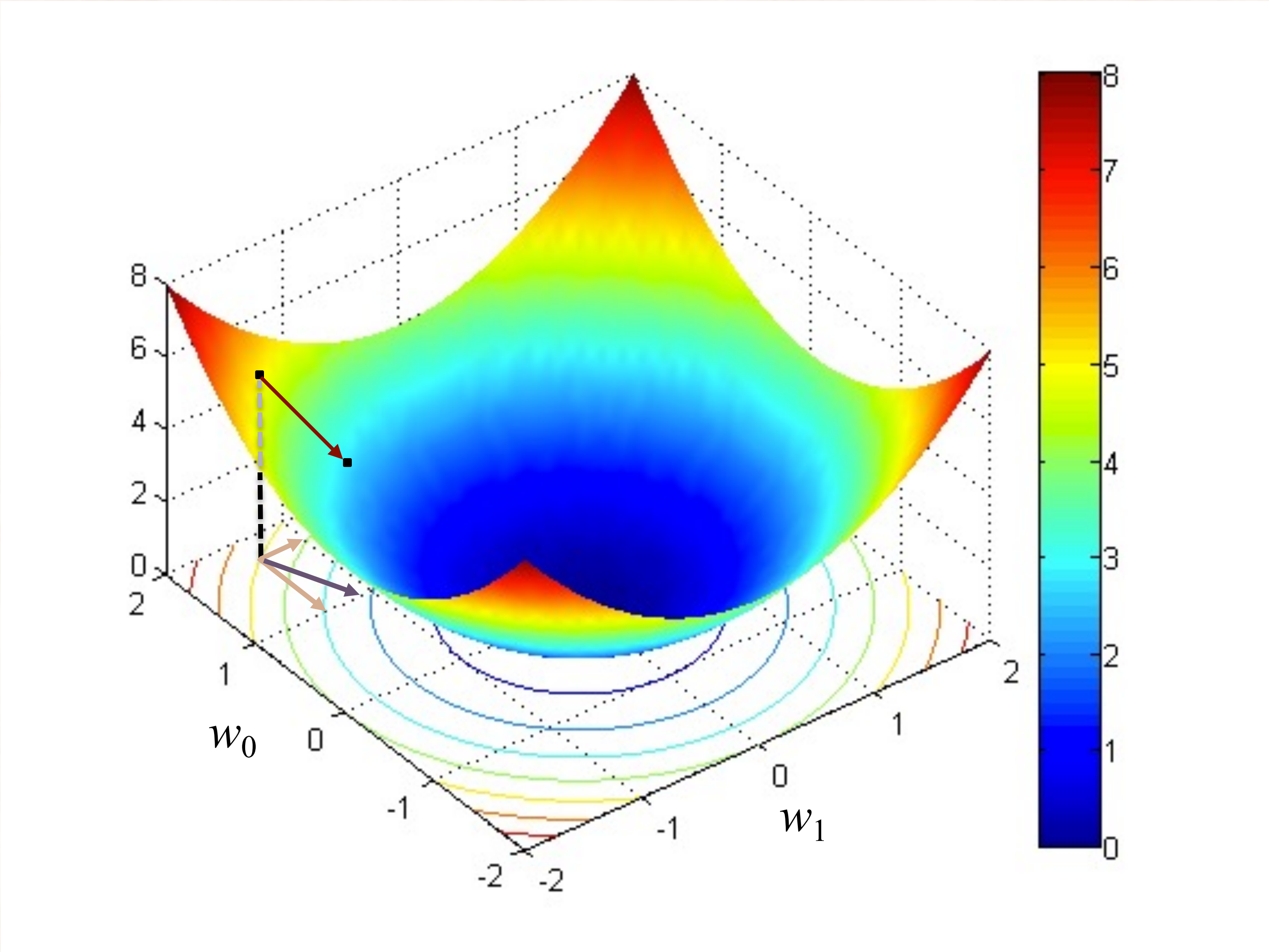
Gradient Descent: Nonconvex Objective



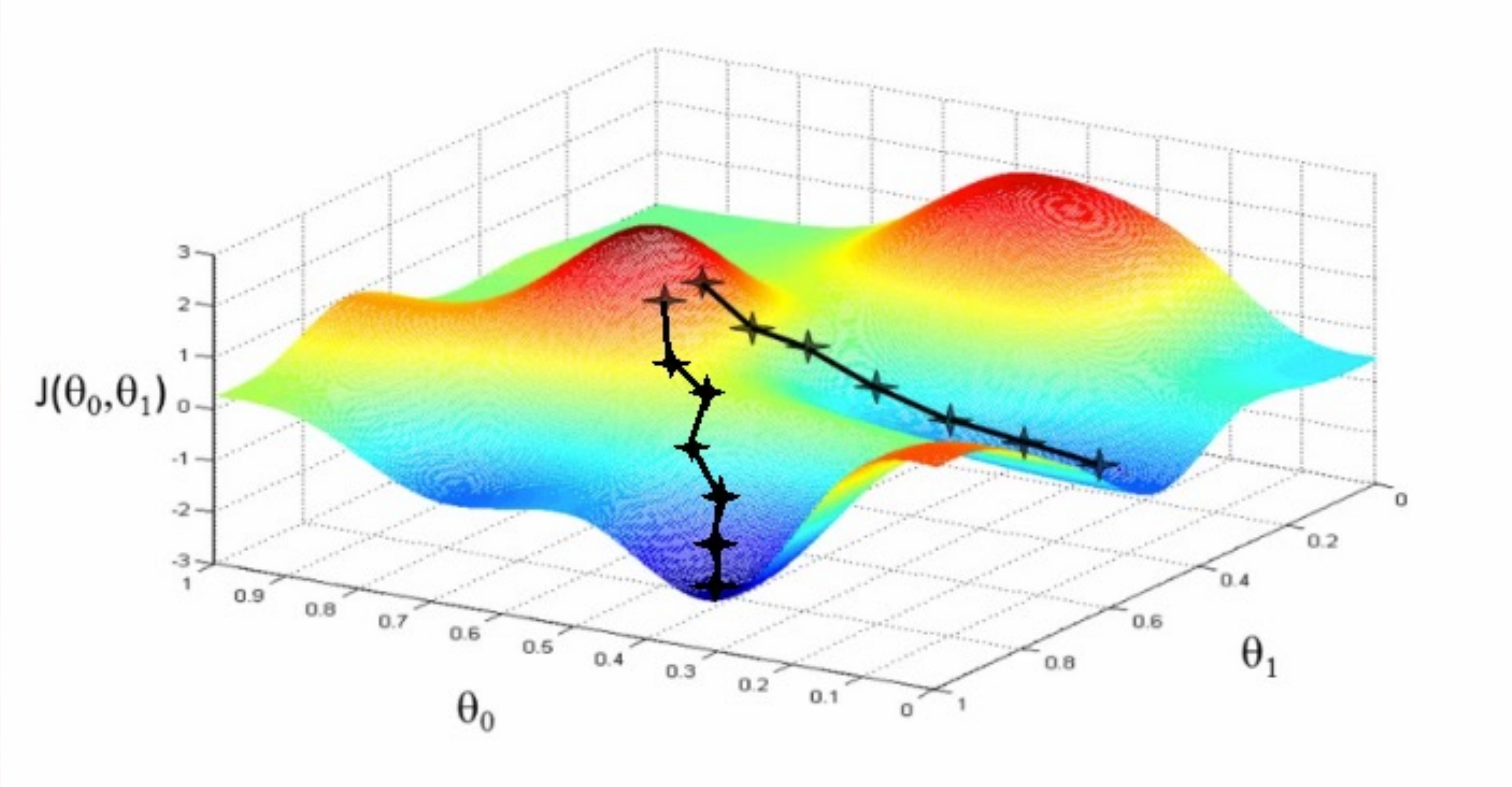
Convex Multivariate Objective



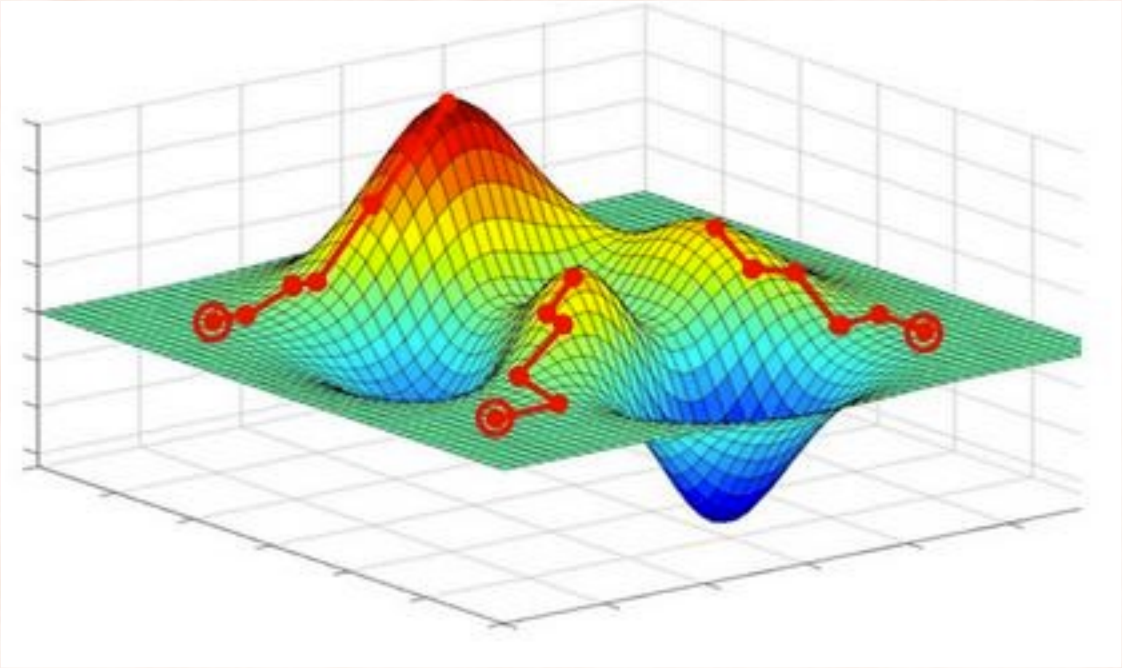
Gradient Step and Contour Lines



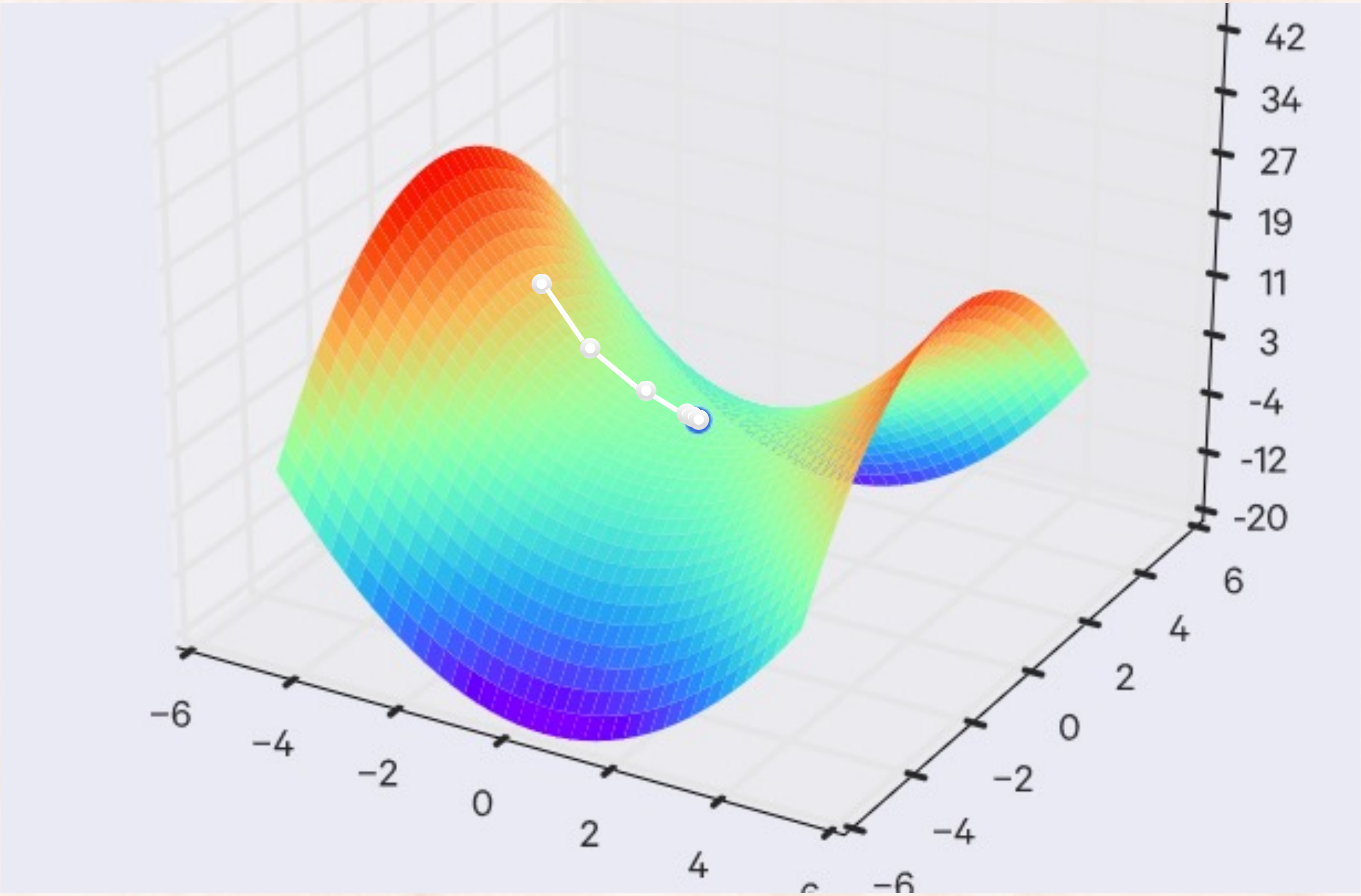
Gradient Descent: Nonconvex Objectives



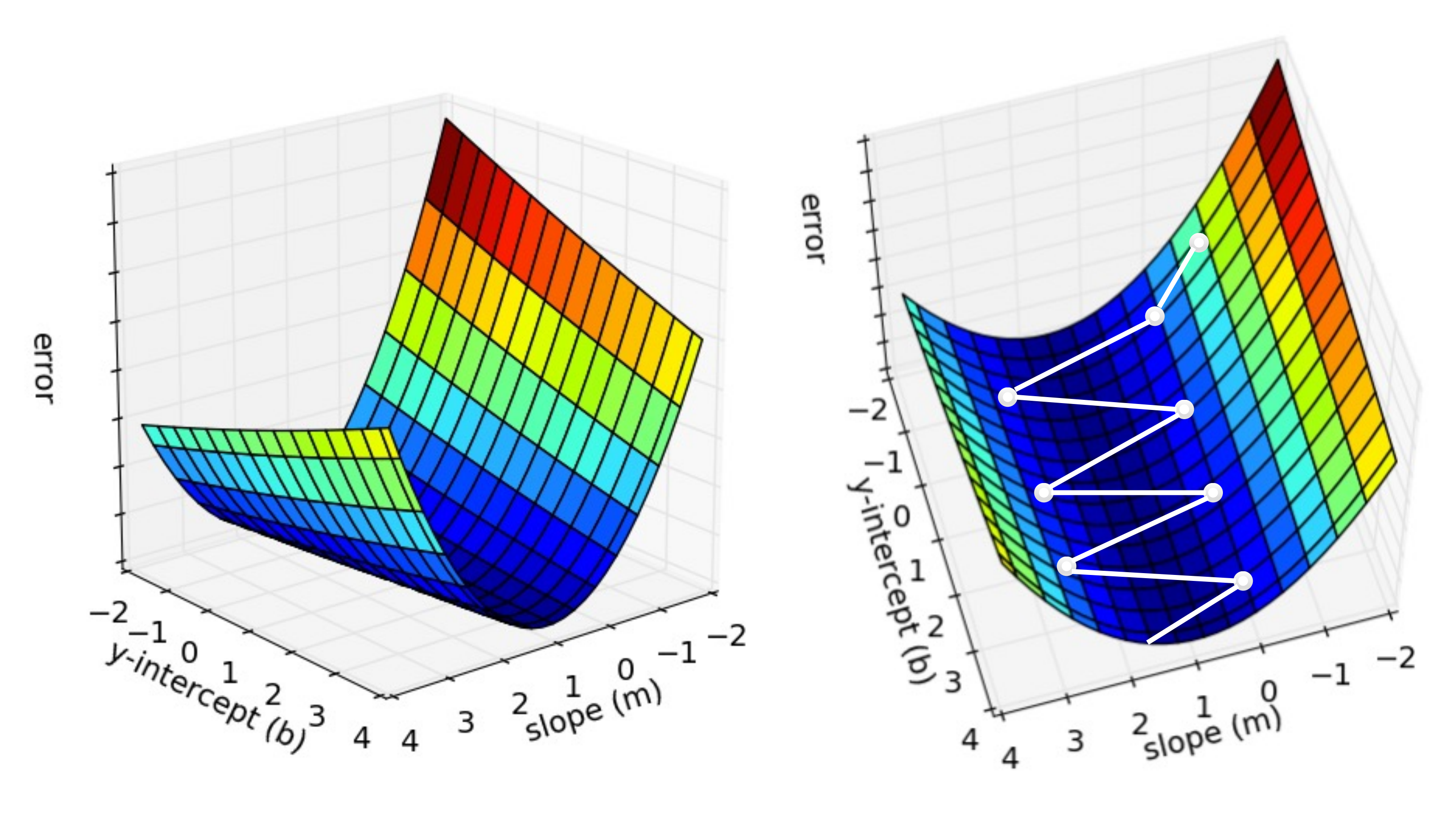
Gradient Descent & Plateaus



Gradient Descent & Saddle Points



Gradient Descent & Ravines



Gradient Descent & Ravines

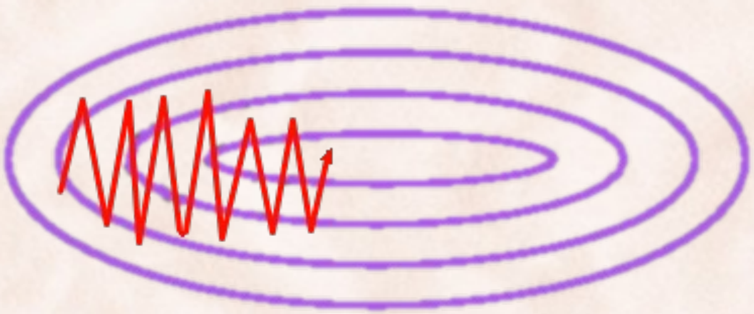
- **Ravines** are areas where the surface curves much more steeply in one dimension than another.
  - Common around local optima.
  - GD oscillates across the slopes of the ravines, making slow progress towards the local optimum along the bottom.
- Use **momentum** to help accelerate GD in the relevant directions and dampen oscillations:
  - Add a fraction of the past **update vector** to the current update vector.
    - The momentum term increases for dimensions whose previous gradients point in the same direction.
    - It reduces updates for dimensions whose gradients change sign.
    - Also <u>reduces the risk of getting stuck in local minima</u>.

Gradient Descent & Momentum

Vanilla Gradient Descent:

$$\mathbf{v}^{\tau+1} = \eta \nabla J(\mathbf{w}^{\tau})$$

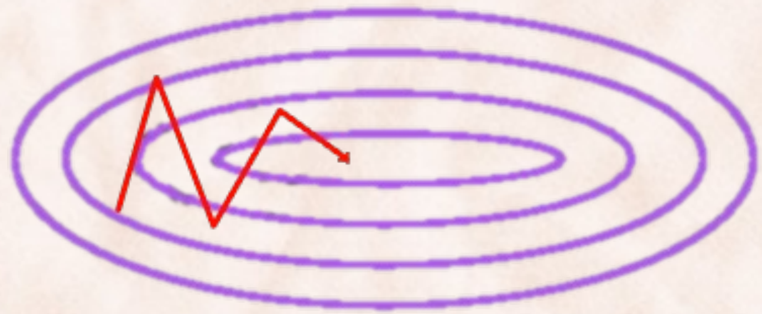
$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



Gradient Descent w/ Momentum:

$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



γ is usually set to 0.9 or similar.

The momentum term increases for dimensions whose gradients point in the same directions and reduces updates for dimensions whose gradients change directions.

Momentum & Nesterov Accelerated Gradient

GD with Momentum:

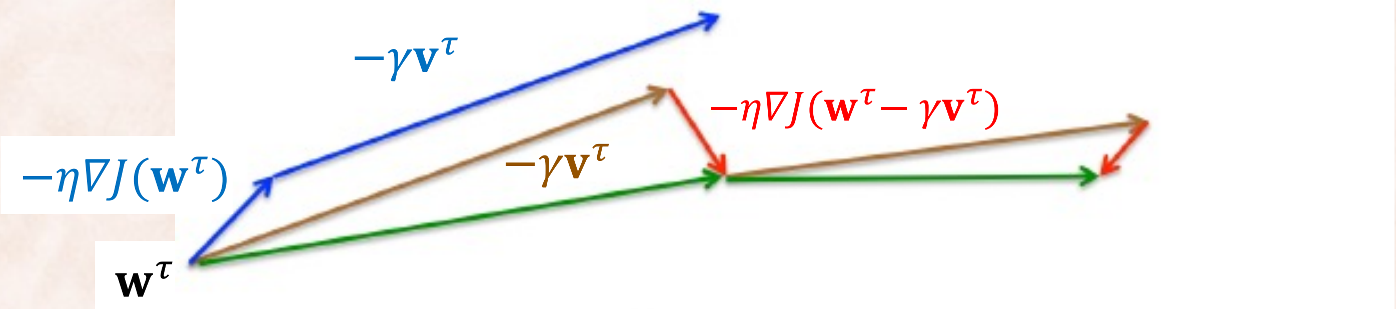
$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$

Nesterov Accelerated Gradient:

$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau} - \gamma \mathbf{v}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



Nesterov update (Source: G. Hinton's lecture 6c)

By making an anticipatory update, NAGs prevents GD from going too fast => significant improvements when training RNNs.

Batch vs. Stochastic Gradient Descent

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$$

- Depending on how much data is used to compute the gradient at each step:
  - **Batch gradient descent**:
    - Use all the training examples.
  - **Stochastic gradient descent** (SGD).
    - Use one training example, update after each.
    - **Minibatch gradient descent**.
      - Use a constant number of training examples (minibatch).

Batch Gradient Descent: Linear Regression

- Sum-of-squares error:

$$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$$

$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right)^2$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \, \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \frac{1}{N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right) \mathbf{x}^{(n)}$$

Stochastic Gradient Descent: Linear Regression

$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$

- Sum-of-squares error:

$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)^2 = \frac{1}{N} \sum_{n=1}^{N} J\left(\mathbf{w}^{\tau}, \mathbf{x}^{(n)}\right)$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \, \nabla J\left(\mathbf{w}^{\tau}, \mathbf{x}^{(n)}\right)$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta\left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right) \mathbf{x}^{(n)}$$

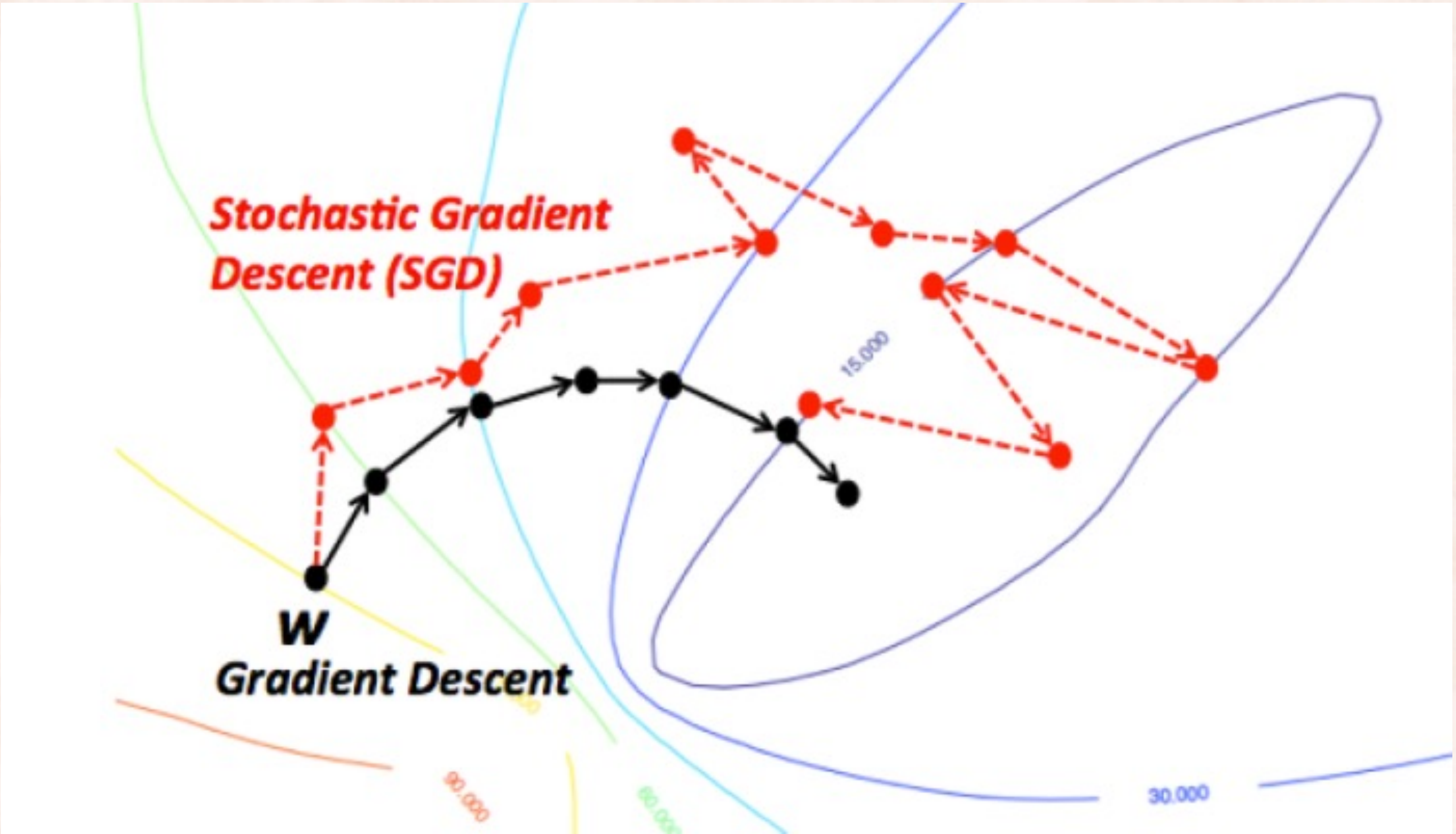
- Update parameters **w** after each example, sequentially:

  => the *least-mean-square* (LMS) algorithm.

Batch GD vs. Stochastic GD

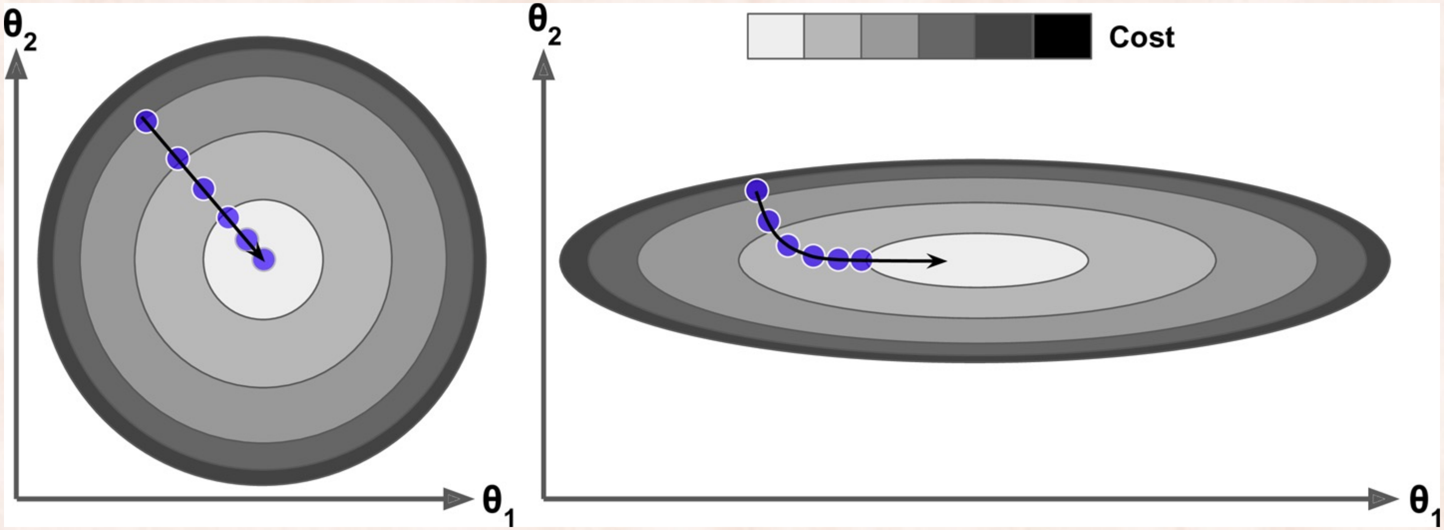
- Accuracy:
- Time complexity:
- Memory complexity:
- Online learning:

Batch GD vs. Stochastic GD



Pre-processing Features

- Features may have very different scales, e.g. x_1 = rooms vs. x_2 = size in sq ft.
  - Right (*different scales*): GD goes first towards the bottom of the bowl, then slowly along an almost flat valley.
  - Left (*scaled features*): GD goes straight towards the minimum.



Feature Scaling

- Scaling between [0, 1] or [−1, +1]:
  - For each feature x_j, compute min_j and max_j **over the training examples**.
  - Scale x_j as follows: $\hat{x}_j = \frac{x_j - min_j}{max_j - min_j}$
- Scaling to standard normal distribution:
  - For each feature x_j, compute sample μ_j and sample σ_j **over the training examples**.
  - Scale x_j as follows: $\hat{x}_j = \frac{x_j - \mu_j}{\sigma_j}$
- **Use the same scaling factors at test time**:
  - Clip to min_j and max_j.

Gradient Descent vs. Normal Equations

- **Gradient Descent**:
  - Need to select learning rate η.
  - May need many iterations:
    - Can do *Early Stopping* on validation data for regularization.
  - Scalable when number of training examples N is large.

- **Normal Equations**:
  - No iterations => easy to code.
  - Computing $(X^T X)^{-1}$ has cubic time complexity => slow for large N.
  - $X^T X$ may be singular:
    1. Redundant (linearly dependent) features.
    2. #features > #examples => do *feature selection* or *regularization*.

Implementation: Vectorization

- **Version 1**: Compute gradient component-wise.

$$\nabla J(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)\mathbf{x}^{(n)}$$

$$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T\mathbf{x}^{(n)}$$

```
grad = np.zeros(K)
for n in range(N):
    h = w.dot(X[:,n]) // This NumPy code assumes examples stored in columns of X.
    temp = h − t[n]
    for k in range(K):
      grad(k) = grad(k) + temp * X[n,k]
for k in range(K):
   grad(k) = grad(k) / N
```

Implementation: Vectorization

- **Version 2**: Compute gradient, partially vectorized.

$$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$$

$$\nabla J(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right) \mathbf{x}^{(n)}$$

```
grad = np.zeros(K)
for n in range(N):                // This NumPy code assumes examples stored in columns of X.
    grad = grad + (w.dot(X[:,n])) − t[n]) * X[:,n]
grad = grad / N
```

Implementation: Vectorization

- **Version 3**: Compute gradient, vectorized.

$$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$$

$$\nabla J(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right) \mathbf{x}^{(n)}$$

grad = X.dot(**w**.dot(X) − **t**) / N

NumPy code above assumes examples stored in columns of X.

Homework: Rewrite to work with examples stored on rows.

Batch Gradient Descent: Ridge Regression

- Sum-of-squares error + regularizer

$h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$

$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \left(\lambda \mathbf{w} + \frac{1}{N} \sum_{n=1}^{N} \left(h_{\mathbf{w}(\mathbf{x}^{(n)})} - t_n\right) \mathbf{x}^{(n)} \right)$$

Implementation: Vectorization

- **Version 3**: Compute gradient, vectorized.

$$\nabla J(\mathbf{w}) = \lambda \mathbf{w} + \frac{1}{N} \sum_{n=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n \right) \mathbf{x}^{(n)} \qquad h_{\mathbf{w}}(\mathbf{x}^{(n)}) = \mathbf{w}^T \mathbf{x}^{(n)}$$

grad = $\lambda *$ **w** + X.dot(**w**.dot(X) − **t**) / N

NumPy code above assumes examples stored in columns of X.

Homework: Rewrite to work with examples stored on rows.

Implementation: Gradient Checking

- Want to minimize $J(\theta)$, where θ is a scalar.

- Mathematical definition of derivative:

$$\frac{d}{d\theta}J(\theta) = \lim_{\varepsilon \to \infty} \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}$$

- Numerical approximation of derivative:

$$\frac{d}{d\theta}J(\theta) \approx \frac{J(\theta+\varepsilon) - J(\theta-\varepsilon)}{2\varepsilon}$$ where $\varepsilon = 0.0001$

Implementation: Gradient Checking

- If $\boldsymbol{\theta}$ is a vector of parameters $\boldsymbol{\theta}_i$,
  - Compute numerical derivative with respect to each $\boldsymbol{\theta}_i$.
  - Aggregate all derivatives into numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$.

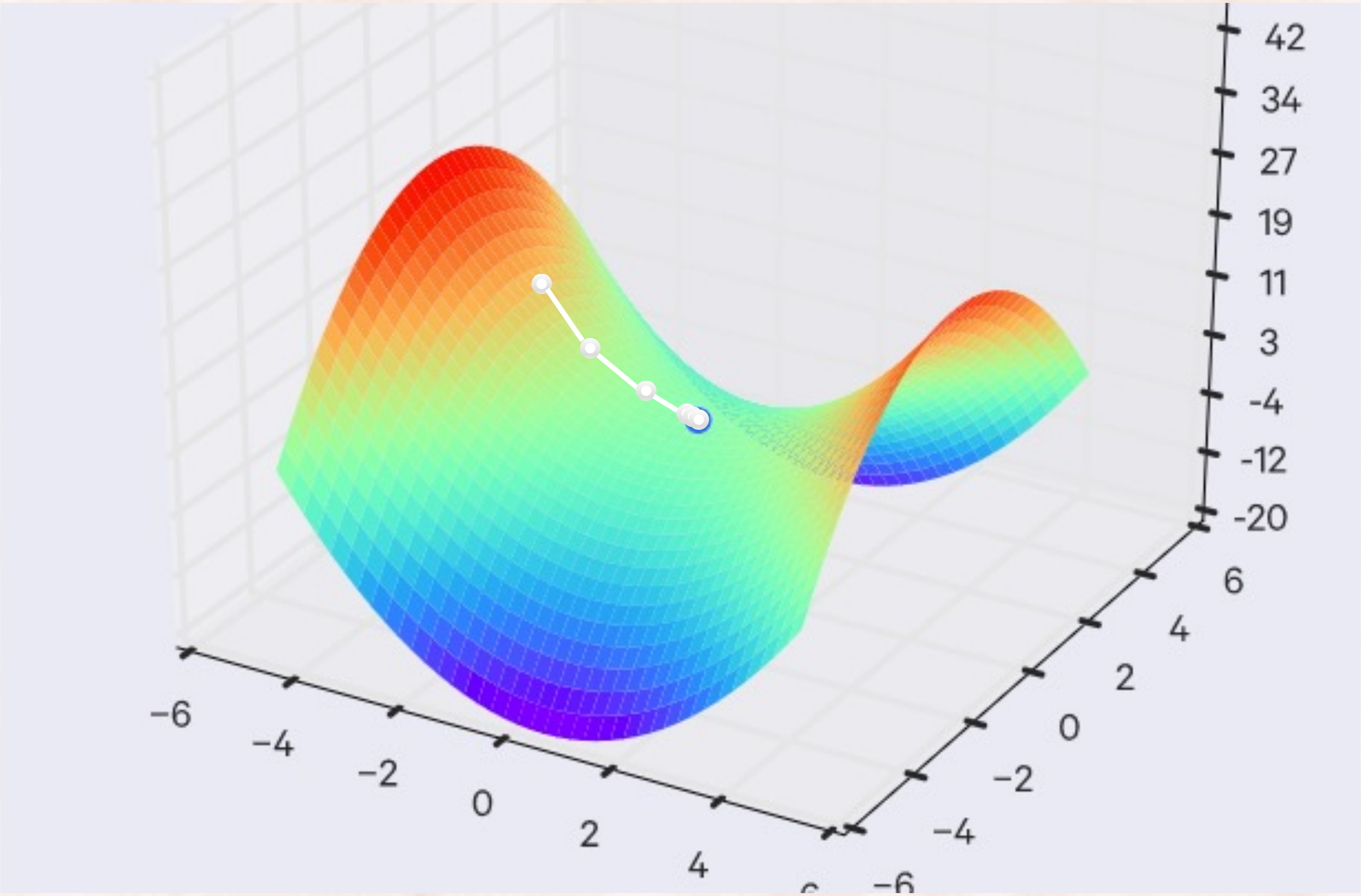
- Compare numerical gradient $G_{\text{num}}(\boldsymbol{\theta})$ with implementation of gradient $G_{\text{imp}}(\boldsymbol{\theta})$:

$$\frac{\left\| G_{num}(\boldsymbol{\theta}) - G_{imp}(\boldsymbol{\theta}) \right\|}{\left\| G_{num}(\boldsymbol{\theta}) + G_{imp}(\boldsymbol{\theta}) \right\|} \leq 10^{-6}$$

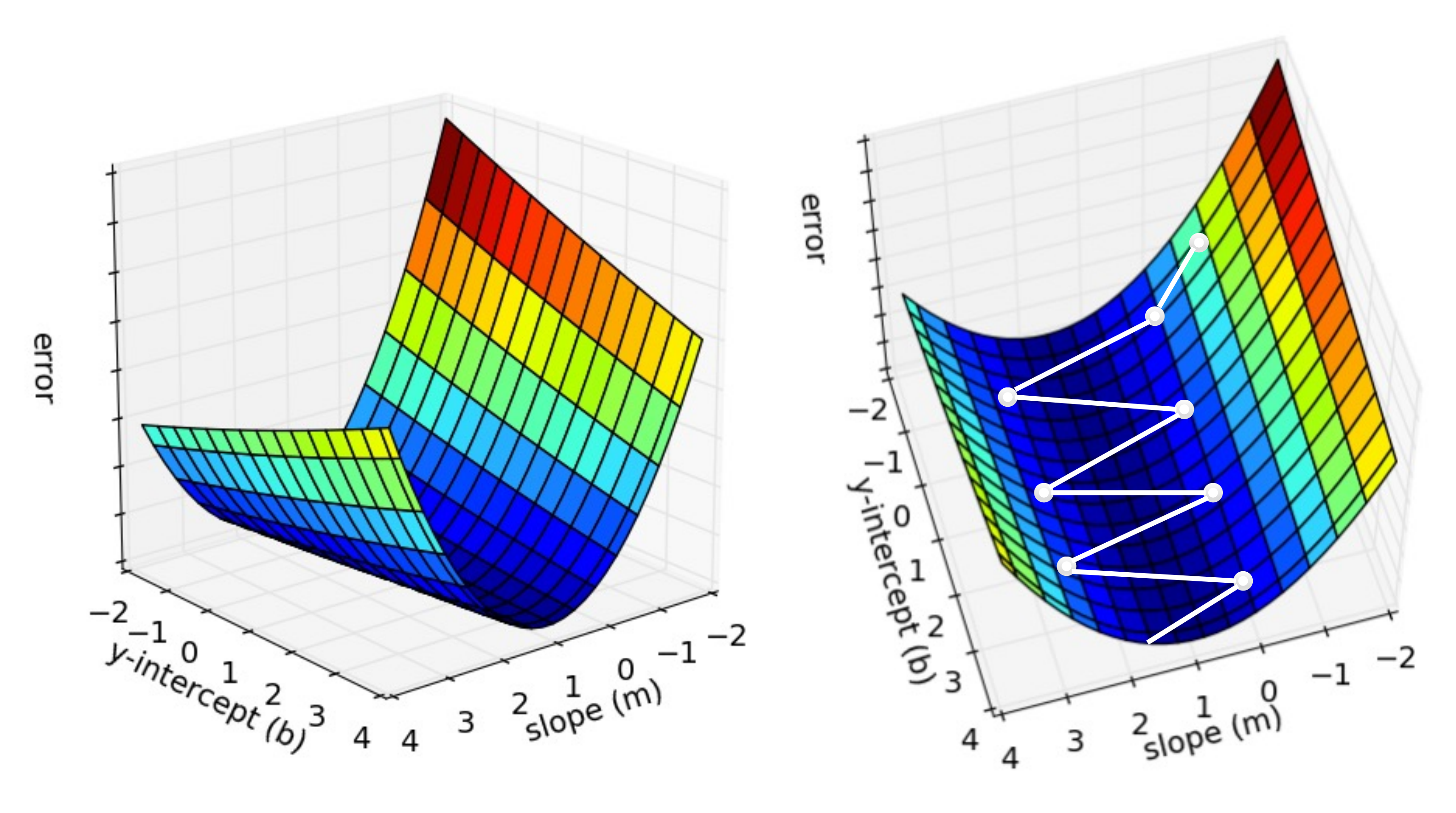
Gradient Descent Optimization Algorithms

- **Momentum**.
- **Nesterov Accelerated Gradient** (NAG).
- Adaptive learning rates methods:
  - Idea is to perform larger updates for infrequent params and smaller updates for frequent params, by accumulating previous gradient values for each parameter.
    - **Adagrad**:
      - Divide update by sqrt of sum of squares of past gradients.
    - **Adadelta**.
    - **RMSProp**.
    - **Adaptive Moment Estimation** (Adam)

Gradient Descent & Saddle Points



Gradient Descent & Ravines



Gradient Descent & Ravines

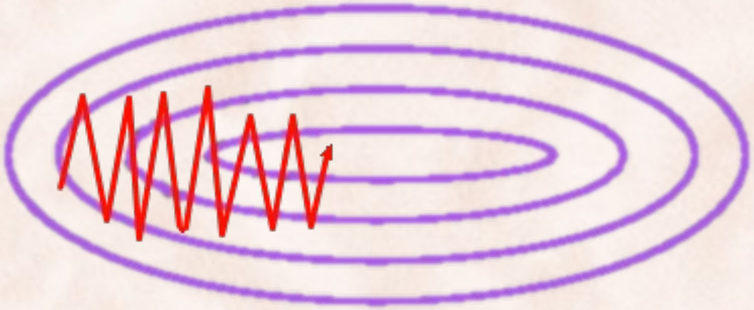
- **Ravines** are areas where the surface curves much more steeply in one dimension than another.
  - Common around local optima.
  - GD oscillates across the slopes of the ravines, making slow progress towards the local optimum along the bottom.
- Use **momentum** to help accelerate GD in the relevant directions and dampen oscillations:
  - Add a fraction of the past **update vector** to the current update vector.
    - The momentum term increases for dimensions whose previous gradients point in the same direction.
    - It reduces updates for dimensions whose gradients change sign.
    - Also reduces the risk of getting stuck in local minima.

Gradient Descent & Momentum

Vanilla Gradient Descent:

$$\mathbf{v}^{\tau+1} = \eta \nabla J(\mathbf{w}^{\tau})$$

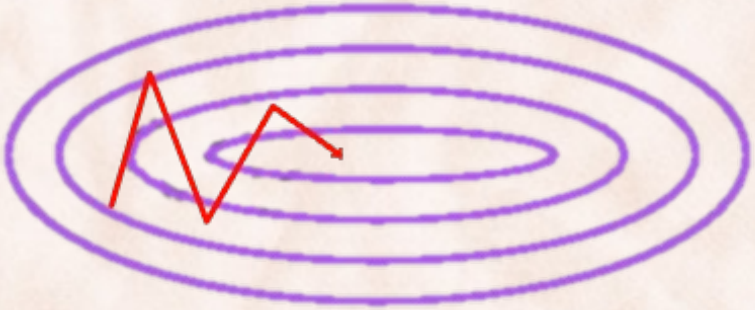
$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



Gradient Descent w/ Momentum:

$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



γ *is usually set to* 0.9 *or similar*.

The momentum term increases for dimensions whose gradients point in the same directions and reduces updates for dimensions whose gradients change directions.

Momentum & Nesterov Accelerated Gradient

GD with Momentum:

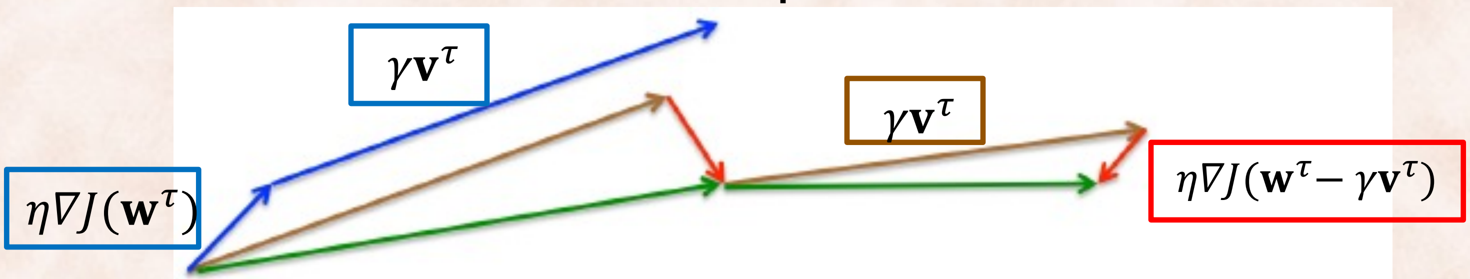
$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$

Nesterov Accelerated Gradient:

$$\mathbf{v}^{\tau+1} = \gamma \mathbf{v}^{\tau} + \eta \nabla J(\mathbf{w}^{\tau} - \gamma \mathbf{v}^{\tau})$$

$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \mathbf{v}^{\tau+1}$$



Nesterov update (Source: G. Hinton's lecture 6c)

By making an anticipatory update, NAGs prevents GD from going too fast => significant improvements when training RNNs.

AdaGrad

- Optimized for problems with sparse features.
- Per-parameter learning rate: make smaller updates for params that are updated more frequently:

$$w_i = w_i - \eta \frac{g_{t,i}}{\sqrt{\epsilon + G_{t,i}}} \quad \text{where } G_{t,i} = \sum_{\tau=1}^{t} g_{\tau,i}^2$$

$$g_{t,i} = \frac{\partial J(\mathbf{w})}{\partial w_i}$$

- Require less tuning of the learning rate compared with SGD.

RMSProp

- Element-wise gradient: $g_i^t = \nabla_{w_i} J(\mathbf{w}_t)$
- Gradient is $\mathbf{g}_t = [g_1^t, g_2^t, \ldots, g_K^t]$
- Element-wise square gradient: $\mathbf{g}_t^2 = \mathbf{g}_t \circ \mathbf{g}_t$

RMSProp:

$$\mathrm{E}_t[\mathbf{g}^2] = \gamma \mathrm{E}_{t-1}[\mathbf{g}^2] + (1-\gamma)\, \mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\eta}{\sqrt{\mathrm{E}_t[\mathbf{g}^2]+\epsilon}} \mathbf{g}_t$$

γ *is usually set to* 0.9, η is set to 0.001

Adam: Adaptive Moment Estimation

- Maintain an exponentially decaying average of past gradients (1st m.) and past squared gradients (2nd m.):
  1) $\mathbf{m}_t = \beta_1 \, \mathbf{m}_{t-1} + (1 - \beta_1) \, \mathbf{g}_t$
  2) $\mathbf{v}_t = \beta_1 \, \mathbf{v}_{t-1} + (1 - \beta_1) \, \mathbf{g}_t^2$

- Biased towards 0 during initial steps, use bias-corrected first and second order estimates:
  1) $\widehat{\mathbf{m}}_t = \frac{\mathbf{m}_t}{1-\beta_1^t}$
  2) $\hat{\mathbf{v}}_t = \frac{\mathbf{v}_t}{1-\beta_2^t}$

Adam: Adaptive Moment Estimation

- First and second moment:

$$\mathbf{m}_t = \beta_1 \, \mathbf{m}_{t-1} + (1 - \beta_1) \, \mathbf{g}_t$$

$$\mathbf{v}_t = \beta_1 \, \mathbf{v}_{t-1} + (1 - \beta_1) \, \mathbf{g}_t^2$$

- Bias-correction:

$$\widehat{\mathbf{m}}_t = \frac{\mathbf{m}_t}{1-\beta_1^t} \text{ and } \hat{\mathbf{v}}_t = \frac{\mathbf{v}_t}{1-\beta_2^t}$$

Adam:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\eta}{\sqrt{\hat{\mathbf{v}}_t} + \epsilon} \widehat{\mathbf{m}}_t$$

Visualization

- Adagrad, RMSprop, Adadelta, and Adam are very similar algorithms that do well in similar circumstances.
  - Insofar, **Adam** might be the best overall choice.