Lecture 5: Training Deep Neural Networks II

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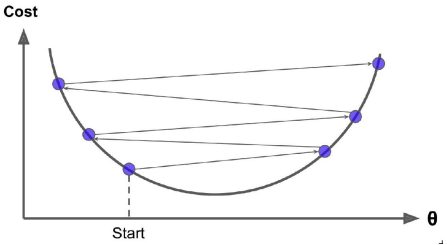
Advanced Machine Learning
September–December 2021

Ill conditioning

- Ill conditioning — small change in input produces a large change in output



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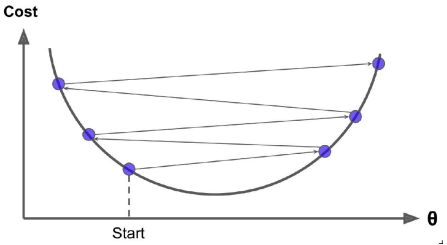

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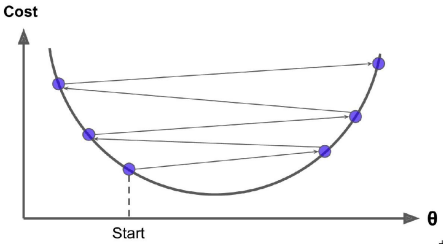

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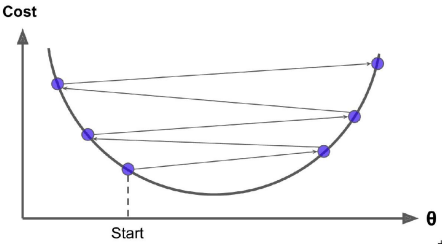

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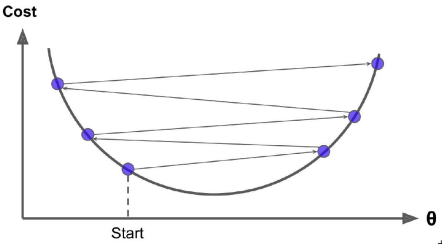

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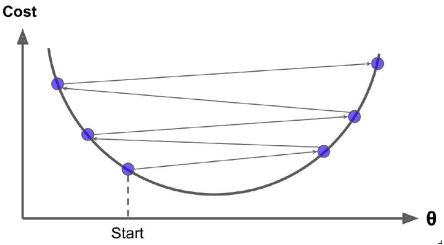

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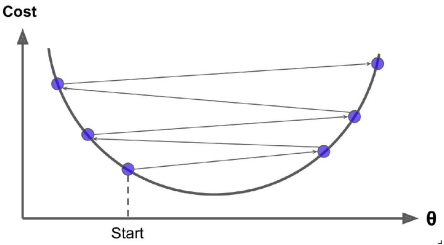
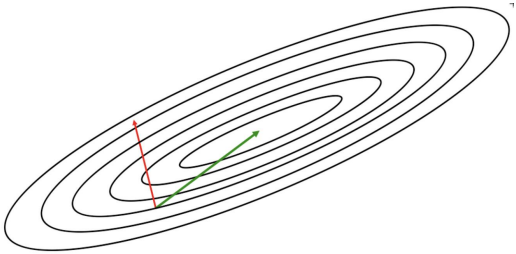
- Analyze H_θ to check for ill conditioning



Directing gradient descent

- Locally steepest direction of descent may be far from the optimum
  - Elliptical contours vs circular contours



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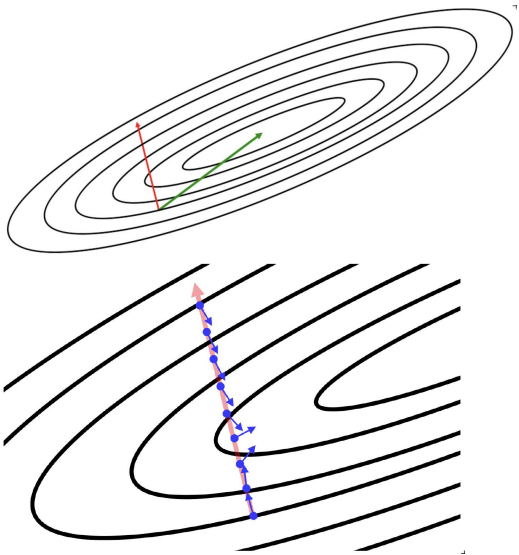

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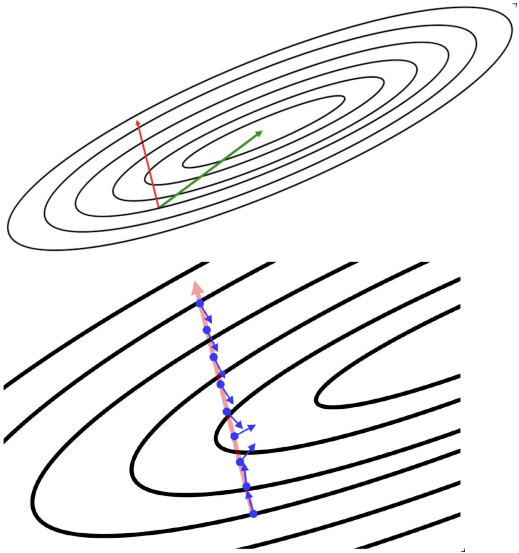
  - Computing Hessian is expensive
  - "Second order" methods are not used in practice



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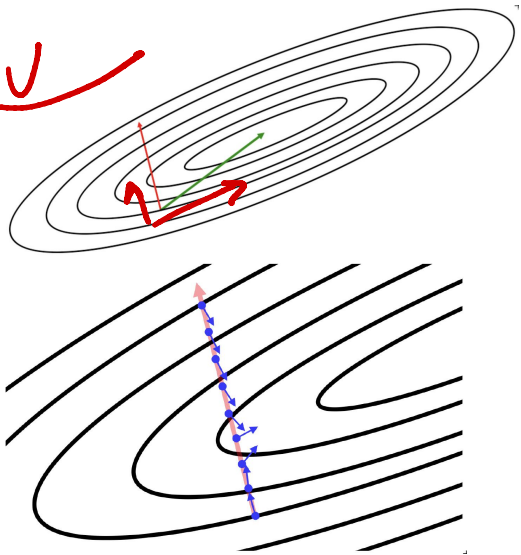
  - "Second order" methods are not used in practice
- Instead, heuristics like momentum and adaptive learning rates



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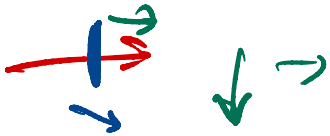
- Introduce velocity v in SGD — assume unit mass
  - Moving average of past gradients, exponential decay
  - If gradient remains steady, velocity increases
- Update rule
  - $v \leftarrow \alpha v - \epsilon \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L(f(x_i; \theta), y_i) \right)$
  - $\theta \leftarrow \theta + v$



$J(\theta)$

$\theta \leftarrow \theta - \epsilon \nabla_\theta J$

$\alpha < 1$

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- Hyperparameter $\alpha \in [0, 1)$ — "friction", exponentially decaying history
  - With constant gradient g, in the limit $\frac{\epsilon g}{1 - \alpha}$, geometric progression

$\alpha = 0.9$

$\frac{1}{1-\alpha} = 10$

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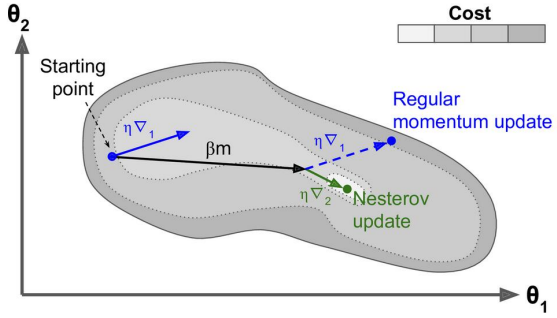
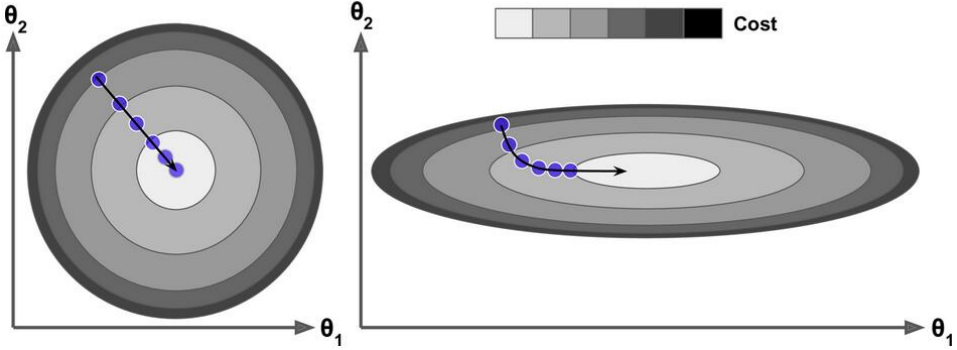
- Controls sideways oscillations better



Adjusting the trajectory

- If features have different scales, gradient descent is steeper in some dimensions
- How can we correct for this?



Adagrad

- Adagrad update rule
  - $g \leftarrow \frac{1}{m} \nabla_\theta \sum_{i=1}^{m} L(f(x_i; \theta), y_i)$
  - $r \leftarrow r + g \cdot g$
  - $\Delta\theta \leftarrow \frac{\epsilon}{\delta + \sqrt{r}} \cdot g$, where $\delta \approx 10^{-7}$, for numerical stability
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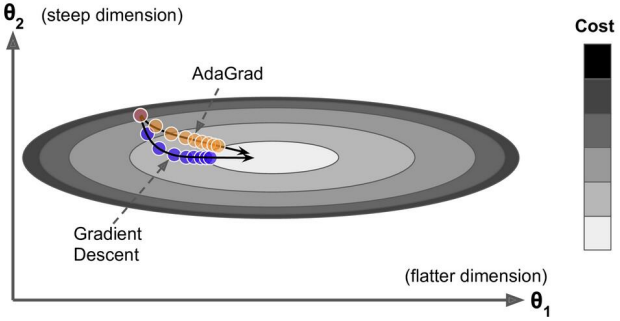

Adaptive learning rates

RMSProp

- Using entire history shrinks learning rate too much
- Exponentially decaying average, discard extreme past
- Update rule
  - $g \leftarrow \frac{1}{m} \nabla_\theta \sum_{i=1}^{m} L(f(x_i; \theta), y_i)$
  - $r \leftarrow \rho r + (1 - \rho)(g \cdot g)$, where ρ is decay rate
  - $\Delta\theta \leftarrow \frac{\epsilon}{\sqrt{\delta + r}} \cdot g$, where $\delta \approx 10^{-6}$
  - $\theta \leftarrow \theta + \Delta\theta$
- New hyperparameter ρ

Adam

- Adaptive moments — combines RMSProp and moments

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- Update rule
  - Step size ϵ; two decay rates ρ_1, ρ_2; two moments, $s = r = 0$; time step $t = 0$
  - $g \leftarrow \frac{1}{m} \nabla_\theta \sum_{i=1}^{m} L(f(x_i; \theta), y_i)$
  - $s \leftarrow \rho_1 s + (1 - \rho_1) g$; $r \leftarrow \rho_2 r + (1 - \rho_2)(g \cdot g)$
  - Correct bias in first and second moments: $\hat{s} \leftarrow \frac{s}{1 - \rho_1^t}$, $\hat{r} \leftarrow \frac{r}{1 - \rho_2^t}$
  - $\Delta\theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r}} + \delta}$; $\theta \leftarrow \theta + \Delta\theta$

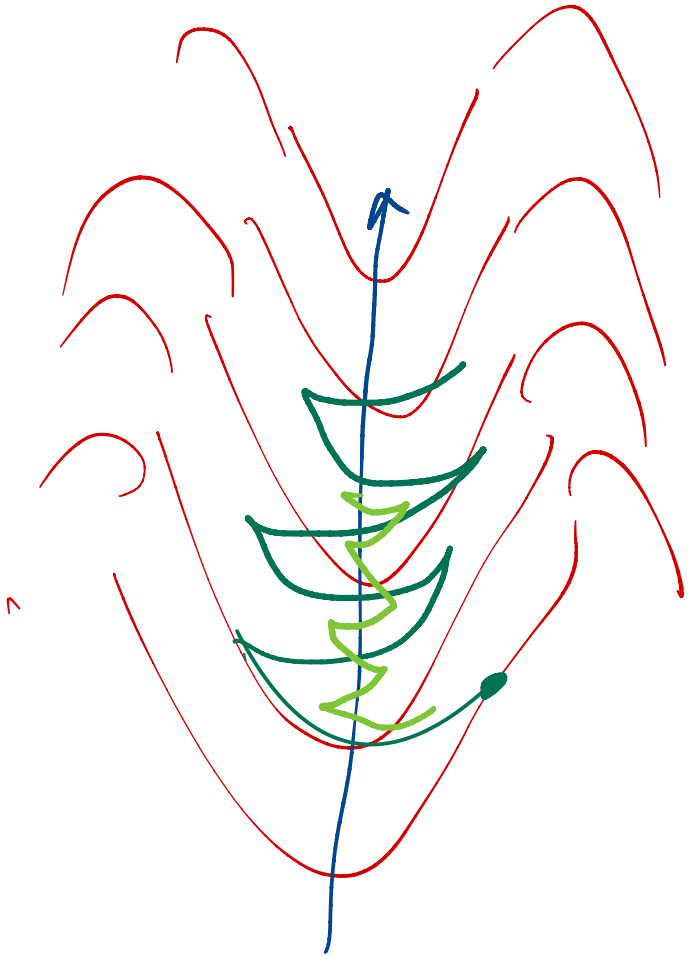
velocity

RMS Prop

$V \leftarrow \alpha V - \epsilon \nabla_\theta J$

$\theta := \theta + V$

Variants on Adam



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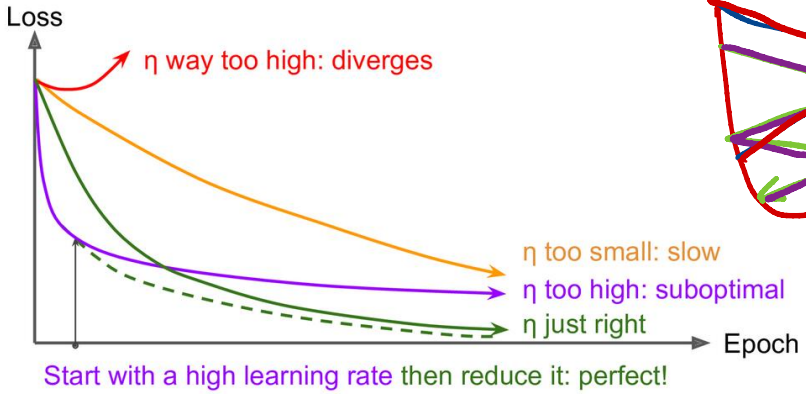
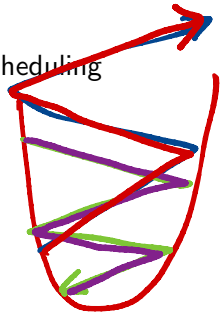
  - $\Delta\theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r}} + \delta}$; $\theta \leftarrow \theta + \Delta\theta$
- No clear theoretical justification for combinining momentum and scaling
- Fairly robust with respect to values of hyperparameters

Adaptive learning rates

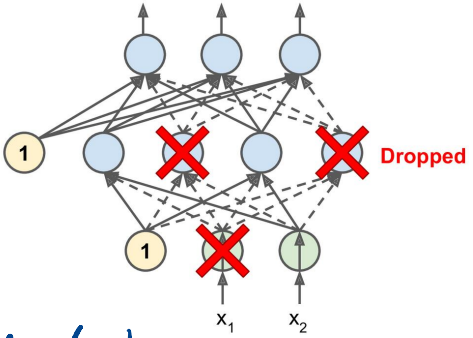
- Choosing a fixed learning rate is hard
- Make a learning rate a function of iteration number
- Power scheduling, exponential scheduling, piecewise constant scheduling





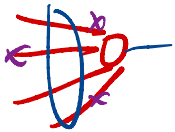
Regularization

- ℓ_1 and ℓ_2 regularization, as usual
- Dropout
  - Disable nodes with probability p
  - Analogy — multifunctional employees
  - Scale weights after training



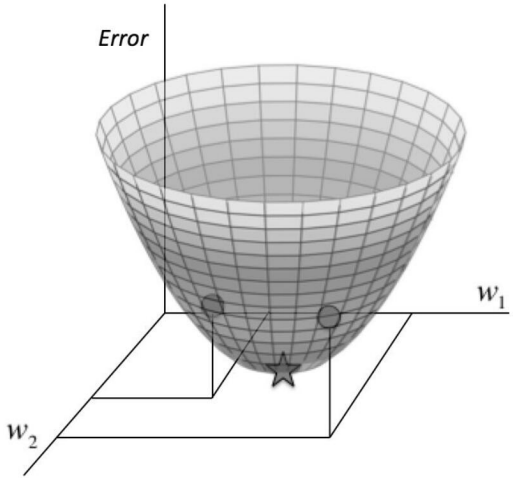
Original Cost + Parameter Cost

Regularization



Local minima

- The loss function for regression is convex
- Gradient descent converges to global optimum



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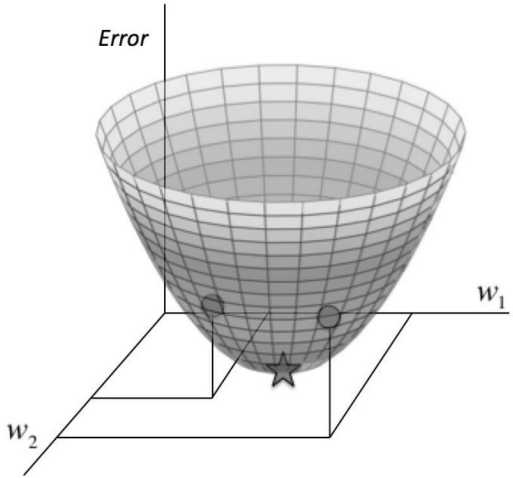

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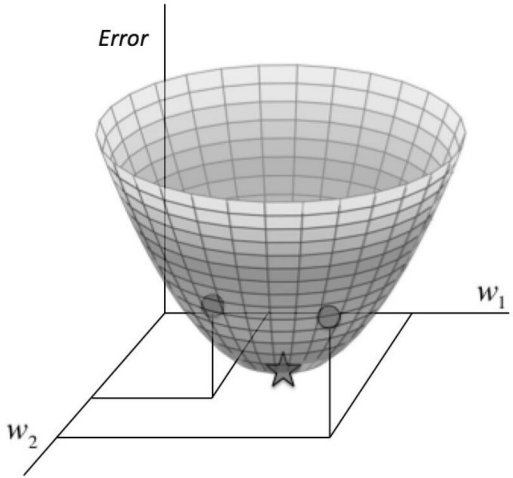

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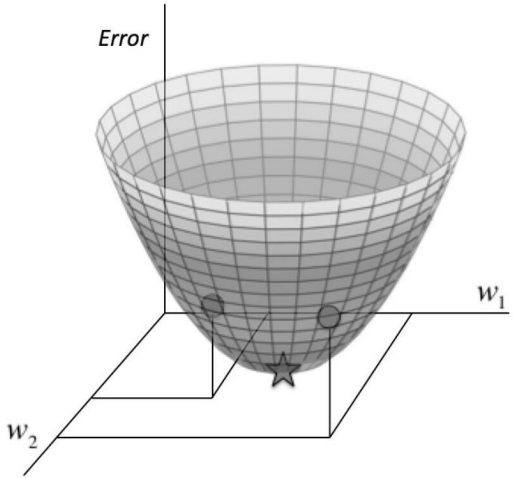
- How does it affect gradient descent?



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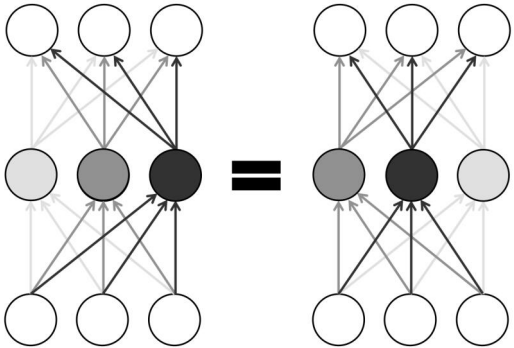

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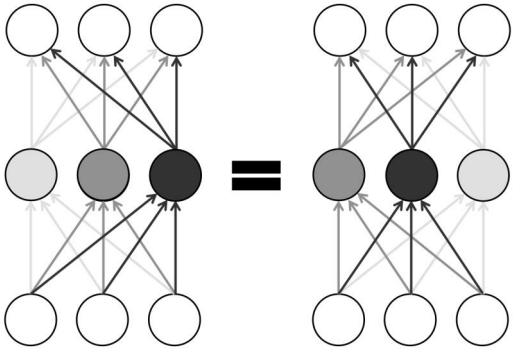

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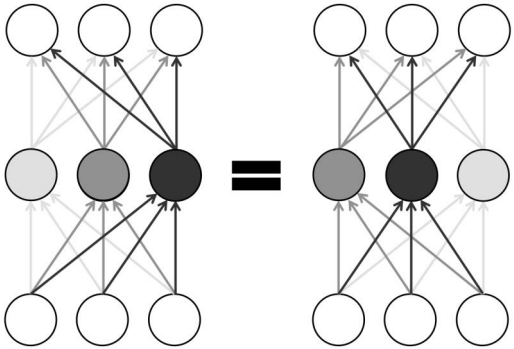
- Large numbers of local minima!



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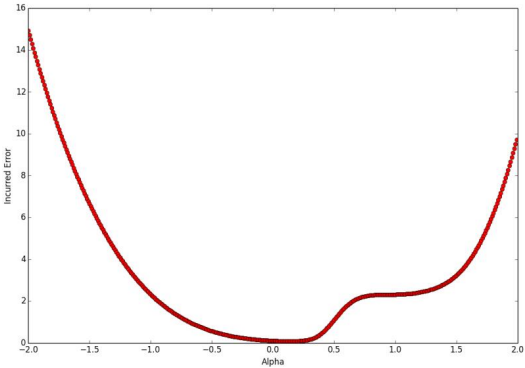

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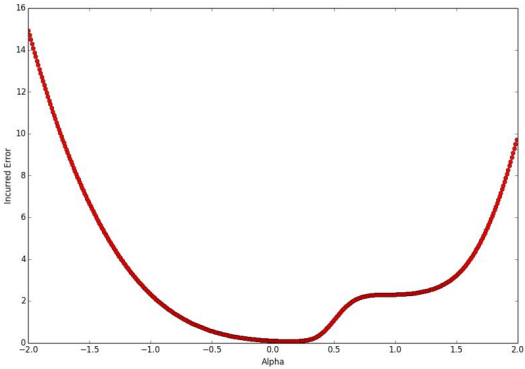

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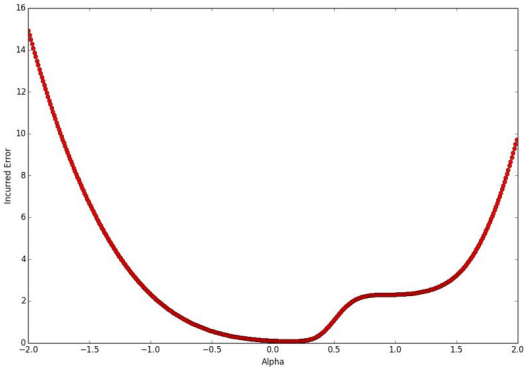
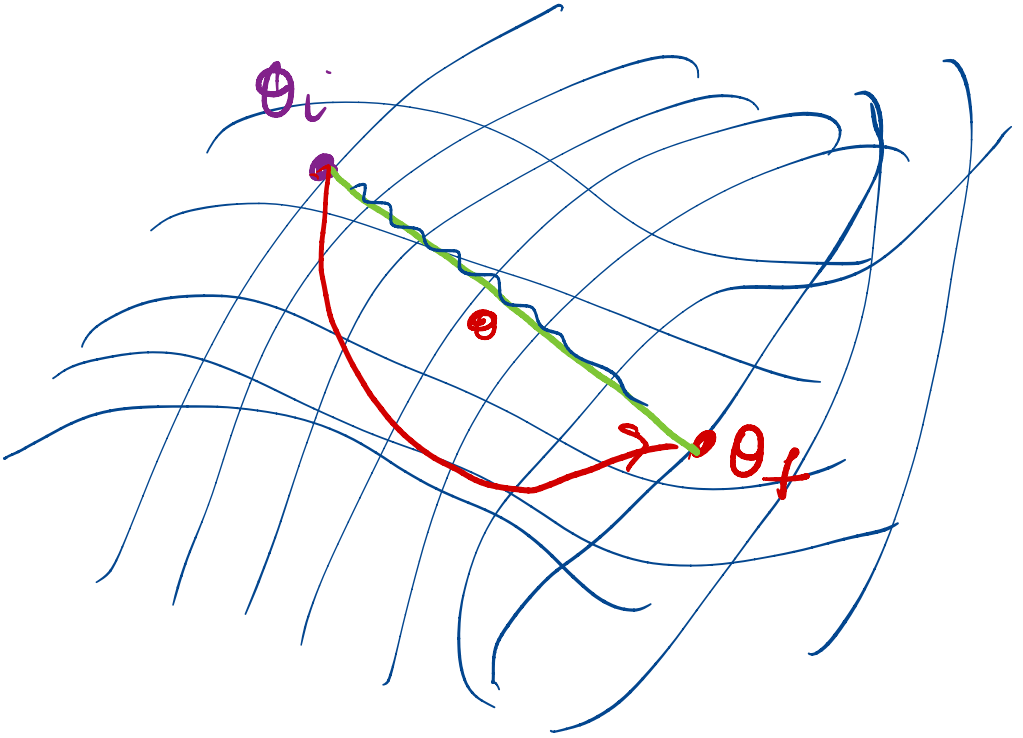
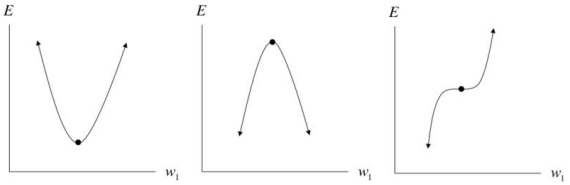
  - Are there problematic local minima along the path?
- Typically, no!




θ_i
θ_f

Saddle points

- Critical points — zero gradient
  - Minimum, maximum or inflection point
  - k critical points $\rightarrow k/3$ are minima



Saddle points

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- In d dimensions
  - Should be minimum in d directions
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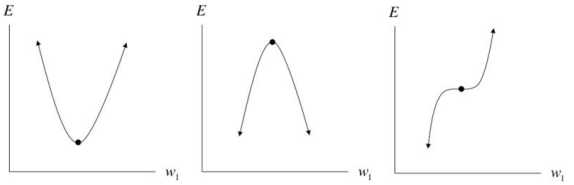

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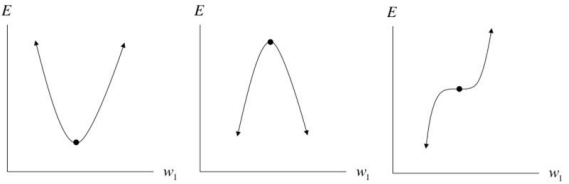

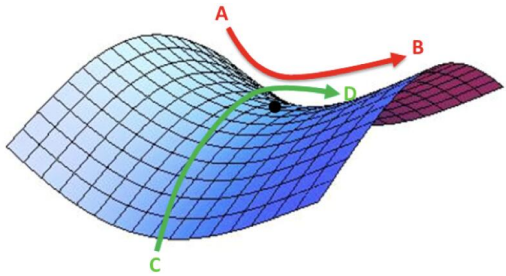

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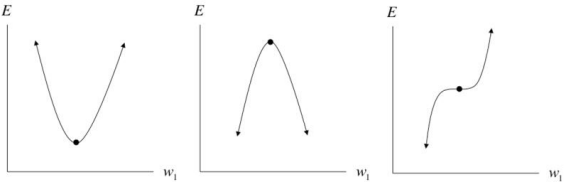

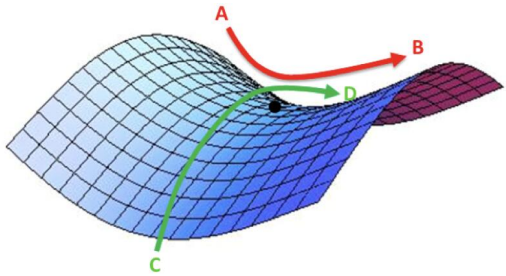

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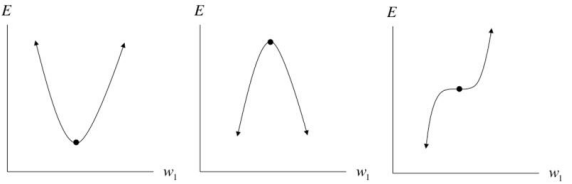

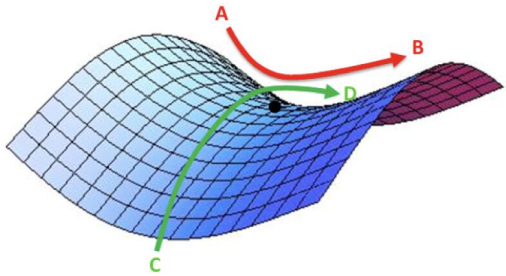

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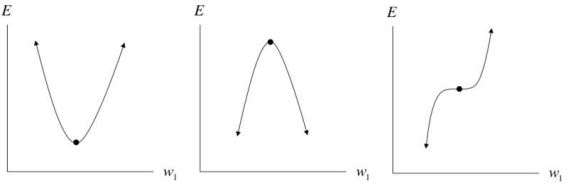

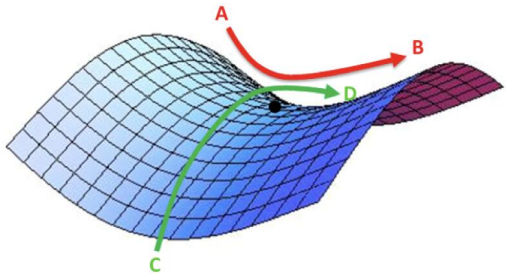

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