Loss Function and Optimization

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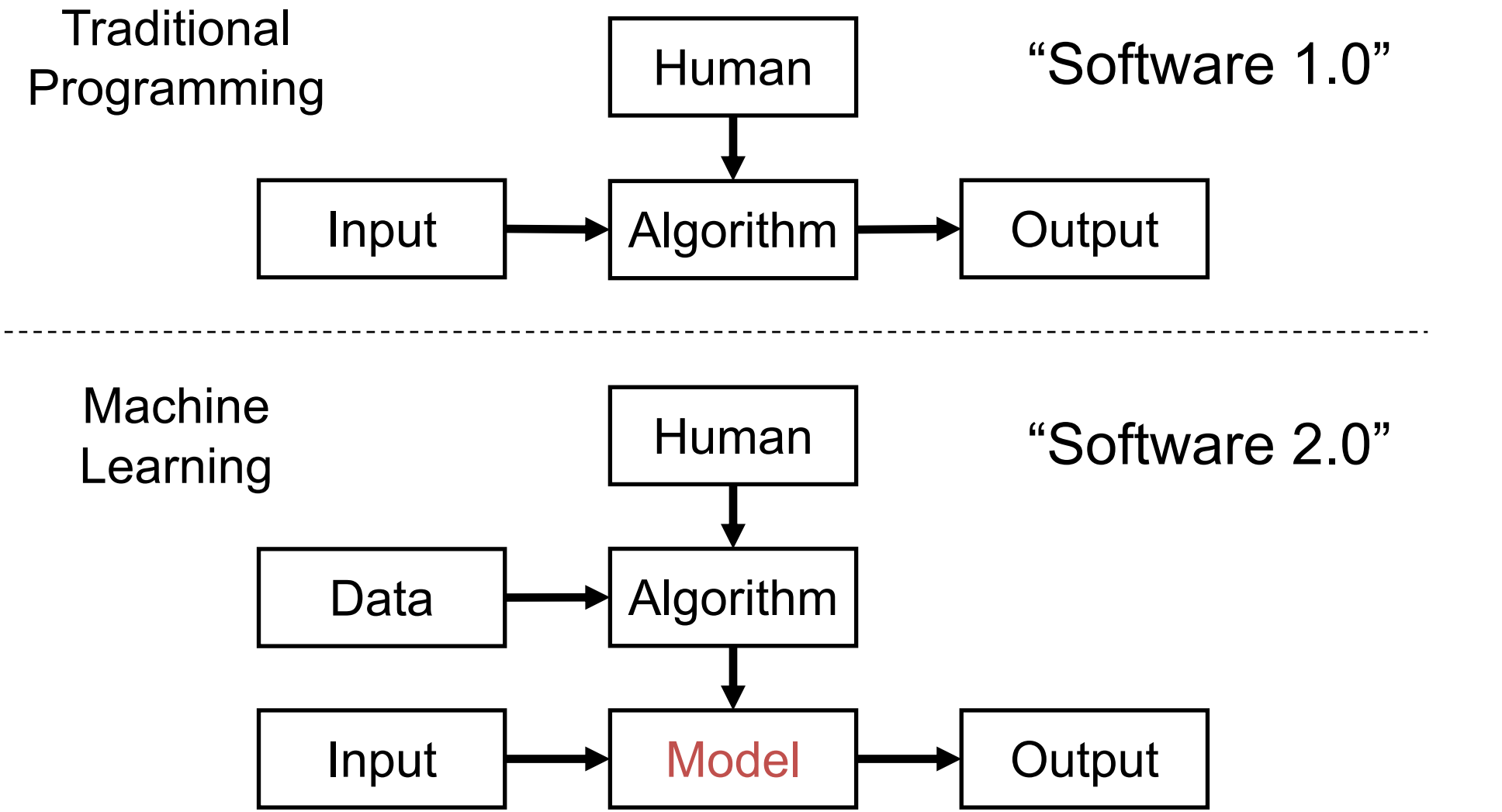
Announcement

- GPU resources for the final project
  - Discovery (your account should be ready to use)
    - try ssh <nu username>@login.discovery.neu.edu
  - Documentation of Discovery: https://rc-docs.northeastern.edu/en/latest/
  - AWS
  - Google could
- Office hour of Prajanan (only this week)
  - Friday, 2-3pm -> Sunday, 10-11pm
- Make-up Office Hour by me (only this week)
  - Friday, 2-3pm
- Project proposal abstract due on Nov 1 (next Monday)

Recap

Machine Learning vs Programming



https://medium.com/@karpathy/software-2-0-a64152b37c35

Slide credit: D Fouhey & J Johnson

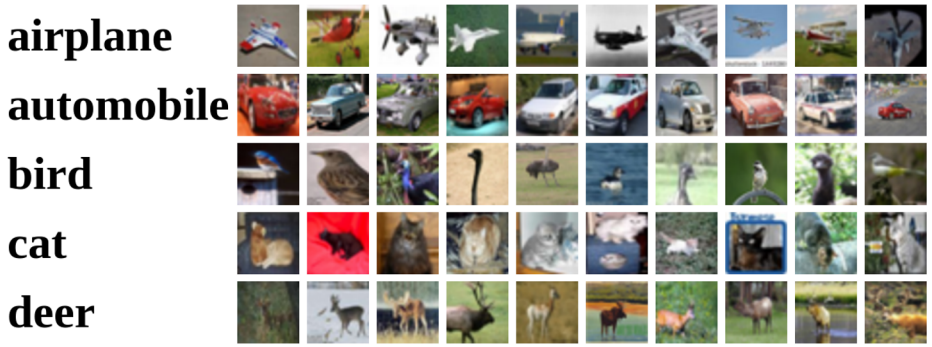
Machine Learning: Data-Driven Approach

1. Collect a large set of data
2. Use Machine Learning to train a model
3. Evaluate the model on new data

```
def train(images, labels):
  # Machine learning!
  return model
```

```
def predict(model, test_images):
  # Use model to predict labels
  return test_labels
```

Example training set



Slide credit: D Fouhey & J Johnson

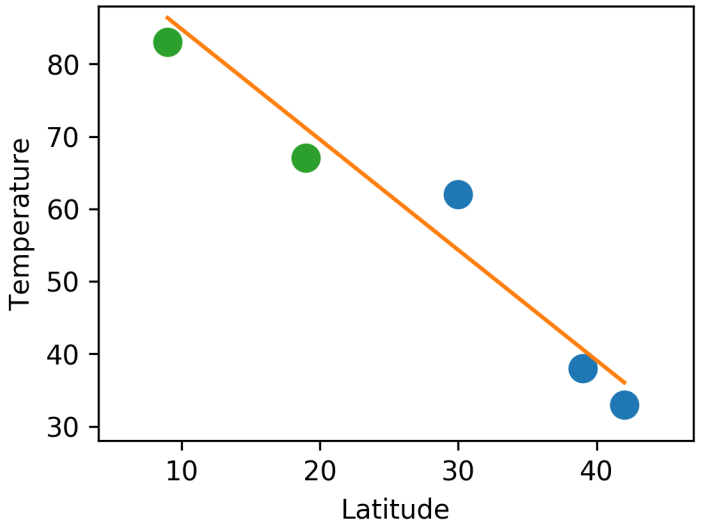
ML Problems in Vision

	Supervised (Inputs+Labels)	**Unsupervised (Just Data)**
Discrete Output	Classification/ Categorization (Object detection, image segmentation)	Clustering
Continuous Output	Regression (stereo disparity, optical flow)	Dimensionality Reduction

Slide adapted from J. Hays

Regularization

	City	Latitude (°)	Temp (F)	No regularization ($\lambda = 0$) Prediction	No regularization ($\lambda = 0$) Error	Regularized ($\lambda = 0.02$) Prediction	Regularized ($\lambda = 0.02$) Error
Train	Ann Arbor	42	33	31.9	1.0	36.0	3.0
	Washington, DC	39	38	39.4	1.4	40.6	2.6
	Austin, TX	30	62	61.7	0.3	54.3	7.7
Test	Mexico City	19	67	88.9	21.9	71.1	4.1
	Panama City	9	83	113.6	30.6	86.4	3.4



L2-Regularized Least Squares

$$\arg\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2 + \lambda\|\boldsymbol{w}\|^2$$

Fit training data — **Regularization Strength** — **Penalize complexity**

Slide credit: D Fouhey & J Johnson

Parameters and Hyperparameters

L2-Regularized Least Squares

$$\arg\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2 + \lambda\|\boldsymbol{w}\|^2$$

Parameter ($\boldsymbol{w}$): (Automatically) selected during training by fitting to training data

Hyperparameter (λ): (Manually) chosen before training, does not depend on training data

Question: How to choose hyperparameters?

Slide credit: D Fouhey & J Johnson

Choosing Hyperparameters

Idea #1: Choose hyperparameters that work best on the data

BAD: λ =0 always works best on training data

Idea #2: Split data into **train** and **test**, choose hyperparameters that work best on test data

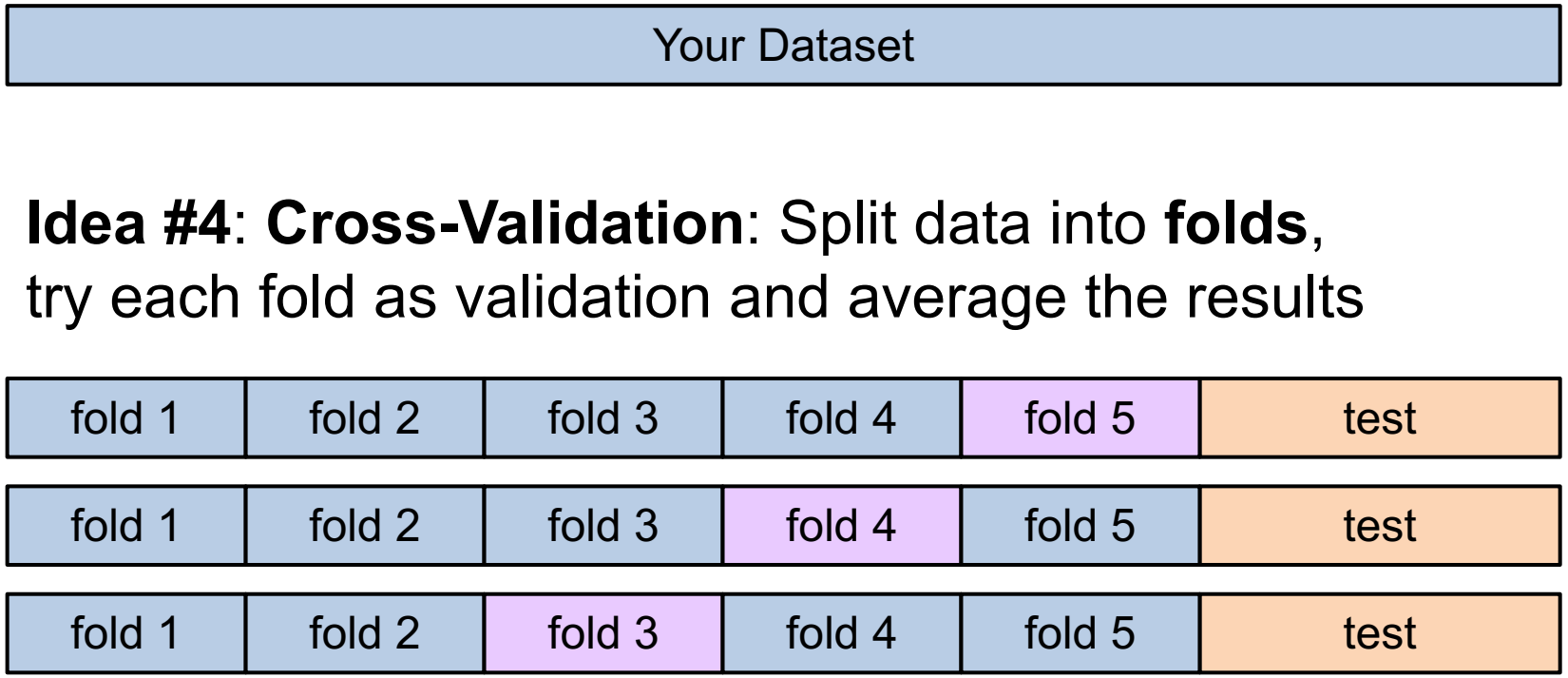
BAD: No idea how we will perform on new data

Idea #3: Split data into **train**, **val**, and **test**; choose hyperparameters on val and evaluate on test

Better!

Slide credit: D Fouhey & J Johnson

Choosing Hyperparameters



Idea #4: **Cross-Validation**: Split data into **folds**, try each fold as validation and average the results

Useful for small datasets, but (unfortunately) not used too frequently in deep learning

Slide credit: D Fouhey & J Johnson

Image Classification: Core Vision Task

Input: image

Output: Assign image to one of a fixed set of categories

cat

bird

deer

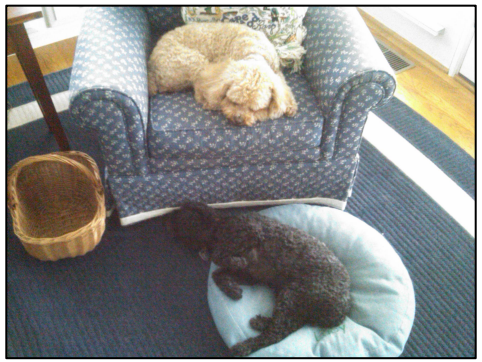
dog

truck

Slide credit: D Fouhey & J Johnson

Linear Classifiers

$\boldsymbol{y_i = wx_i + b,}$ $\boldsymbol{x_i \in \mathbb{R}^D}$ is image feature


Model – one weight per class: $\boldsymbol{w_0, w_1, w_2}$

$\boldsymbol{w_0^T x}$ big if cat

$\boldsymbol{w_1^T x}$ big if dog

$\boldsymbol{w_2^T x}$ big if hippo

Stack together: $\boldsymbol{W_{3xD}}$

Slide credit: D Fouhey & J Johnson

Choosing W: Loss Function

A **loss function** tells how good our current classifier is

Low loss = good classifier
High loss = bad classifier

(Also called: **objective function**; **cost function**)

Given a dataset

$$\{(x_i, y_i)\}_{i=1}^{N}$$

of images x_i and labels y_i,

Loss for a single example is:

$$L_i(f(x_i, W), y_i)$$

Loss for the dataset is

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)$$

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores
$s = f(x_i, W)$

cat	**3.2**
car	5.1
frog	-1.7

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$s = f(x_i, W)$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

cat	**3.2**
car	5.1
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Unnormalized log-probabilities / logits

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

Probabilities must be >= 0

cat	**3.2**	exp →	**24.5**
car	5.1		164
frog	-1.7		0.18

Unnormalized log-probabilities / logits

unnormalized probabilities

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

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$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

	Unnormalized log-probabilities / logits	exp	Probabilities must be >= 0 unnormalized probabilities	normalize	Probabilities must sum to 1 probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164		0.87
frog	-1.7		0.18		0.00

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

Loss

$$L_i = -\log(p_{y_i})$$

	Unnormalized log-probabilities / logits	exp	unnormalized probabilities (Probabilities must be >= 0)	normalize	probabilities (Probabilities must sum to 1)
cat	**3.2**		**24.5**		**0.13**
car	5.1		164		0.87
frog	-1.7		0.18		0.00

$L_i = -\log(0.13)$

$= \mathbf{2.04}$

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$$s = f(x_i, W)$$

Softmax function

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Loss

$$L_i = -\log(p_{y_i})$$

	Unnormalized log-probabilities / logits	exp	Probabilities must be >= 0	normalize	Probabilities must sum to 1
cat	**3.2**		**24.5**		**0.13**
car	5.1		164		0.87
frog	-1.7		0.18		0.00
			unnormalized probabilities		probabilities

$L_i = -\log(0.13)$
$= \mathbf{2.04}$

Maximum Likelihood Estimation
Choose weights to maximize the likelihood of the observed data

Slide credit: D Fouhey & J Johnson

Today's Class

- Loss Function (quantify how good the model's output are compared to the labels)
  - A bit more about cross-entropy loss
  - SVM (hinge) loss
- Optimization (how to efficiently finding the parameters that minimize the loss function)
  - Gradient descent
  - SGD

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

Loss

$$L_i = -\log(p_{y_i})$$

	Unnormalized log-probabilities / logits	exp	Probabilities must be >= 0 unnormalized probabilities	normalize	Probabilities must sum to 1 probabilities	Compare	Correct probs
cat	**3.2**		**24.5**		**0.13**		**1.00**
car	5.1		164		0.87		0.00
frog	-1.7		0.18		0.00		0.00

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

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$$s = f(x_i, W)$$

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Loss

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	Unnormalized log-probabilities / logits	exp	unnormalized probabilities	normalize	probabilities	Compare	Correct probs
	Probabilities must be >= 0				Probabilities must sum to 1		
cat	**3.2**		**24.5**		**0.13**		**1.00**
car	5.1		164		0.87		0.00
frog	-1.7		0.18		0.00		0.00
					Q		P

Cross-Entropy:

$$H(P, Q) = -\sum_y P(y) \log Q(y)$$

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

Want to interpret raw classifier scores as **probabilities**

Classifier scores

$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

Loss

$$L_i = -\log(p_{y_i})$$

cat	**3.2**
car	5.1
frog	-1.7

Putting it all together:

$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

Slide credit: D Fouhey & J Johnson

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cat	**3.2**
car	5.1
frog	-1.7

Putting it all together:

$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

Q: What is the min / max possible loss L_i?

Slide credit: D Fouhey & J Johnson

Cross-Entropy Loss

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Classifier scores

$$s = f(x_i, W)$$

Softmax function

$$p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}$$

Loss

$$L_i = -\log(p_{y_i})$$

cat	**3.2**
car	5.1
frog	-1.7

Putting it all together:

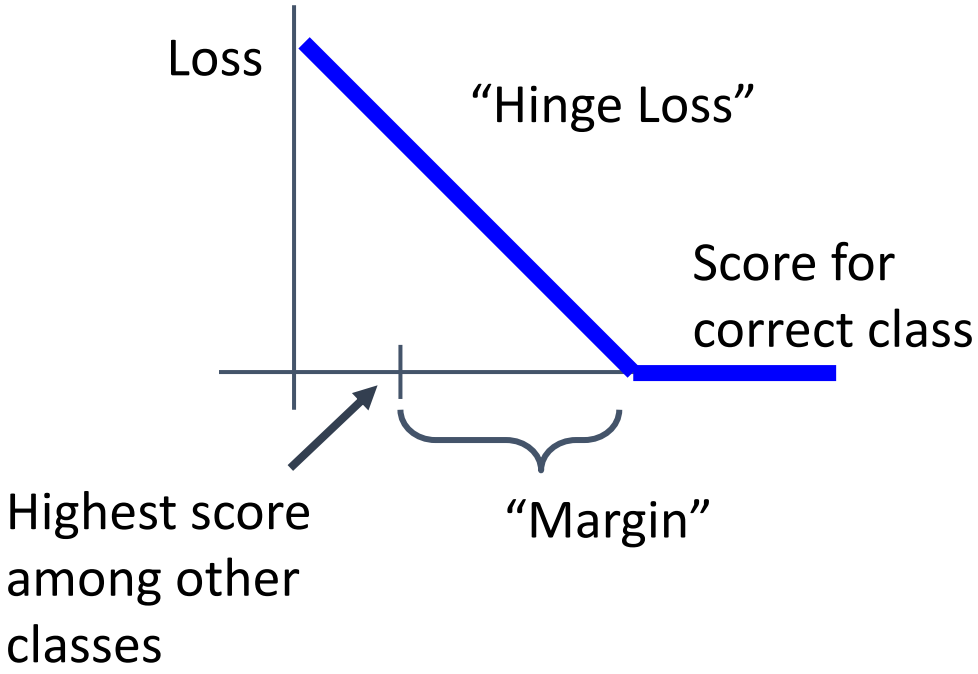
$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

Q: If all scores are small random values, what is the loss?

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss

”The score of the correct class should be higher than all the other scores”



Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

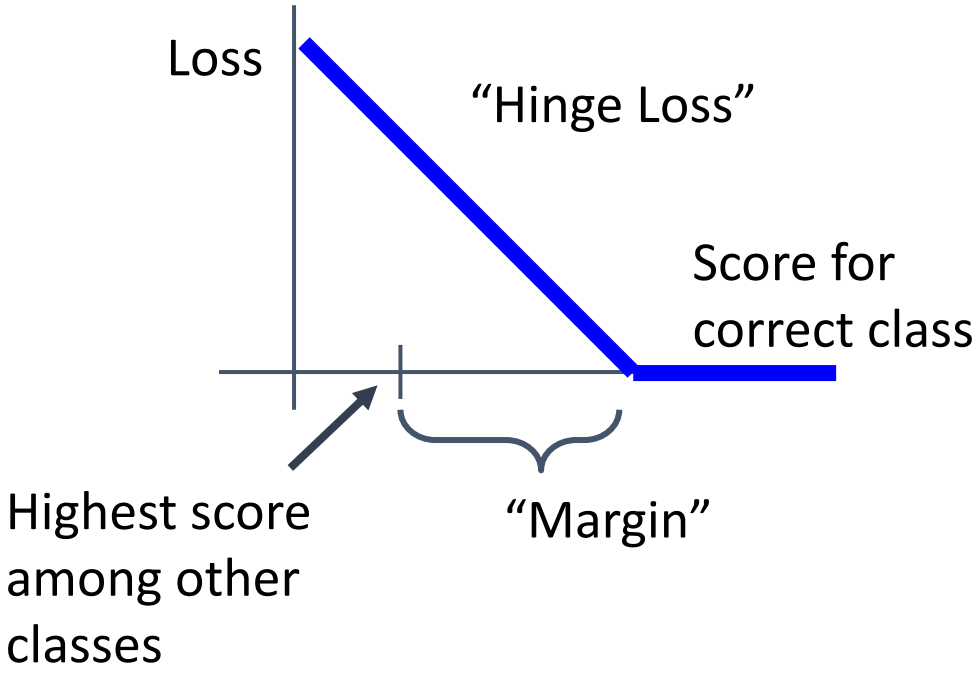
Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss

"The score of the correct class should be higher than all the other scores"



Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

margin

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

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Multiclass SVM Loss



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Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9		

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 5.1 - 3.2 + 1)
+ max(0, -1.7 - 3.2 + 1)
= max(0, 2.9) + max(0, -3.9)
= 2.9 + 0
= 2.9

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 2.2 - (-3.1) + 1)
+max(0, 2.5 - (-3.1) + 1)
= max(0, 6.3) + max(0, 6.6)
= 6.3 + 6.6
= 12.9

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
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frog	-1.7	2.0	**-3.1**
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Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Loss over the dataset is:

L = (2.9 + 0.0 + 12.9) / 3
= 5.27

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



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frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: What happens to the loss if the scores for the car image change a bit?

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

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Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: What are the min and max possible loss?

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
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Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: At initialization W is small so all s ≈ 0. What is the loss?

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: What would happen if sum were over all classes? (including $j = y_i$)

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: What if the loss used mean instead of sum?

Slide credit: D Fouhey & J Johnson

Multiclass SVM Loss



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Loss	2.9	0	12.9

Given an example (x_i, y_i)
(x_i is image, y_i is label)

Let $s = f(x_i, W)$ be scores

Then the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: What if we used this loss instead?

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)^2$$

Slide credit: D Fouhey & J Johnson

Cross-Entropy vs SVM Loss

$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Assume scores:

[10, -2, 3]

[10, 9, 9]

[10, -100, -100]

and $y_i = 0$

Q: What is cross-entropy loss? What is SVM loss?

A: Cross-entropy loss > 0
SVM loss = 0

Slide credit: D Fouhey & J Johnson

Cross-Entropy vs SVM Loss

$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Assume scores:

[10, -2, 3]

[10, 9, 9]

[10, -100, -100]

and $y_i = 0$

Q: What happens to each loss if I slightly change the scores of the last datapoint?

A: Cross-entropy loss will change; SVM loss will stay the same

Slide credit: D Fouhey & J Johnson

Cross-Entropy vs SVM Loss

$$L_i = -\log \frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Assume scores:

[20, -2, 3]

[20, 9, 9]

[20, -100, -100]

and $y_i = 0$

Q: What happens to each loss if I double the score of the correct class from 10 to 20?

A: Cross-entropy loss will decrease, SVM loss still 0

Slide credit: D Fouhey & J Johnson

There is a “bug” with the hinge loss:

$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

E.g. Suppose that we found a W such that L = 0. Is this W unique?

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	12.9

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Before:

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

With W twice as large:

= max(0, 2.6 - 9.8 + 1)
+max(0, 4.0 - 9.8 + 1)
= max(0, -6.2) + max(0, -4.8)
= 0 + 0
= 0

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

An example:

What is the loss? (POLL)

cat	1.3
car	**2.5**
frog	2.0

Loss:

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

An example:

What is the loss?

cat	1.3
car	**2.5**
frog	2.0
Loss:	0.5

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

cat	1.3
car	**2.5**
frog	2.0
Loss:	0.5

An example:

What is the loss?

How could we change W to eliminate the loss? (POLL)

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:

What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:

What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

Wait a minute! Have we done anything useful???

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

$$f(x, W) = Wx$$

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:

What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

Wait a minute! Have we done anything useful???

No! Any example that used to be wrong is still wrong (on the wrong side of the boundary). Any example that is right is still right (on the correct side of the boundary).

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

Regularization

λ = regularization strength (hyperparameter)

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from having too much flexibility.

Simple examples

L2 regularization: $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

Optimization

Goal: find the **w** minimizing some loss function L.

$$\arg\min_{\boldsymbol{w}\in R^D} L(\boldsymbol{w})$$

Works for lots of different Ls:

$$L(\boldsymbol{W}) = \boldsymbol{\lambda}\|\boldsymbol{W}\|_{\boldsymbol{2}}^{\boldsymbol{2}} + \sum_{i=1}^{n} -\log\left(\frac{\exp((Wx)_{y_i})}{\sum_k \exp((Wx)_k))}\right)$$

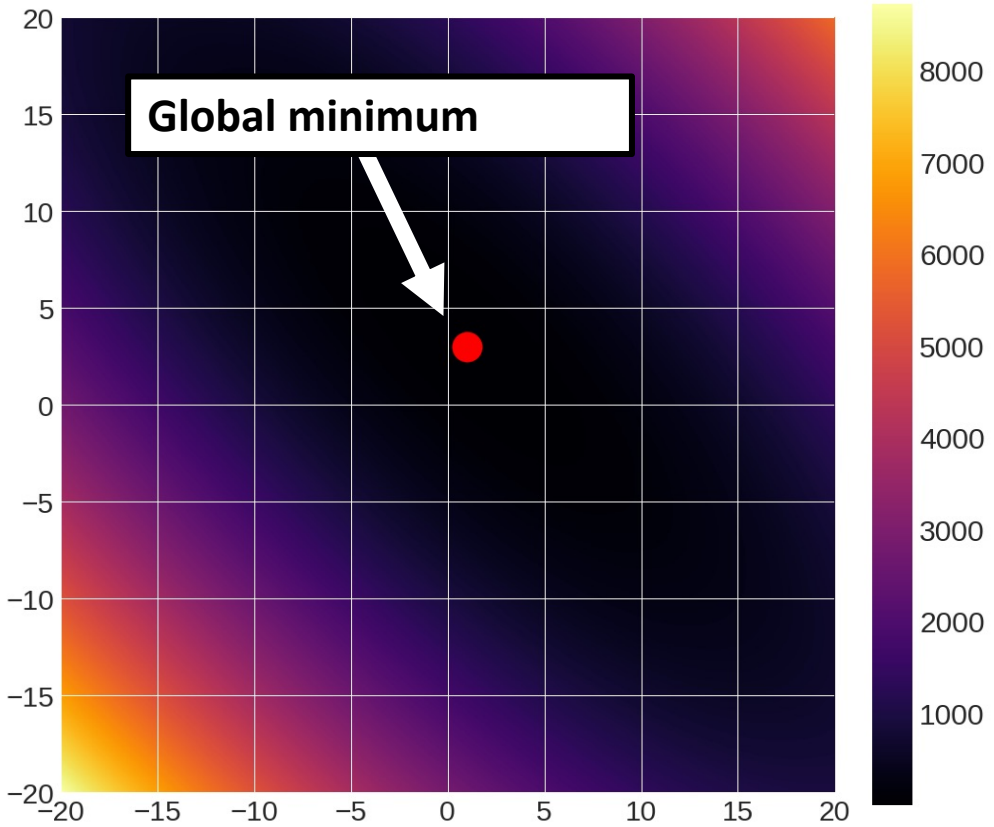
$$L(\boldsymbol{w}) = C\|\boldsymbol{w}\|_2^2 + \sum_{i=1}^{n} \max(0, 1 - y_i \boldsymbol{w}^T \boldsymbol{x_i})$$

$$L(\boldsymbol{w}) = \lambda\|\boldsymbol{w}\|_2^2 + \sum_{i=1}^{n} \left(y_i - \boldsymbol{w^T x_i}\right)^2$$

Slide credit: D Fouhey & J Johnson

Sample Function to Optimize

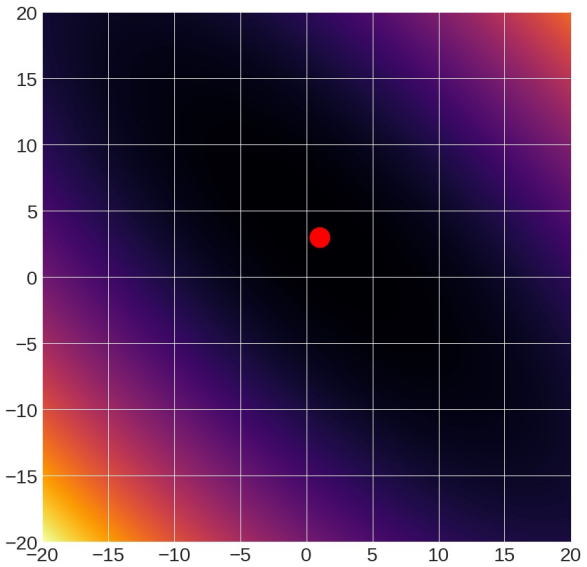
$$f(x,y) = (x+2y-7)^2 + (2x+y-5)^2$$



Warning: This is 2D, intuition may not generalize to high dimension

Slide credit: D Fouhey & J Johnson

Optimization: A Caveat



- Each point in the picture is a function evaluation
- Here it takes microseconds – so we can easily see the answer
- Functions we want to optimize may take hours to evaluate

Slide credit: D Fouhey & J Johnson

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

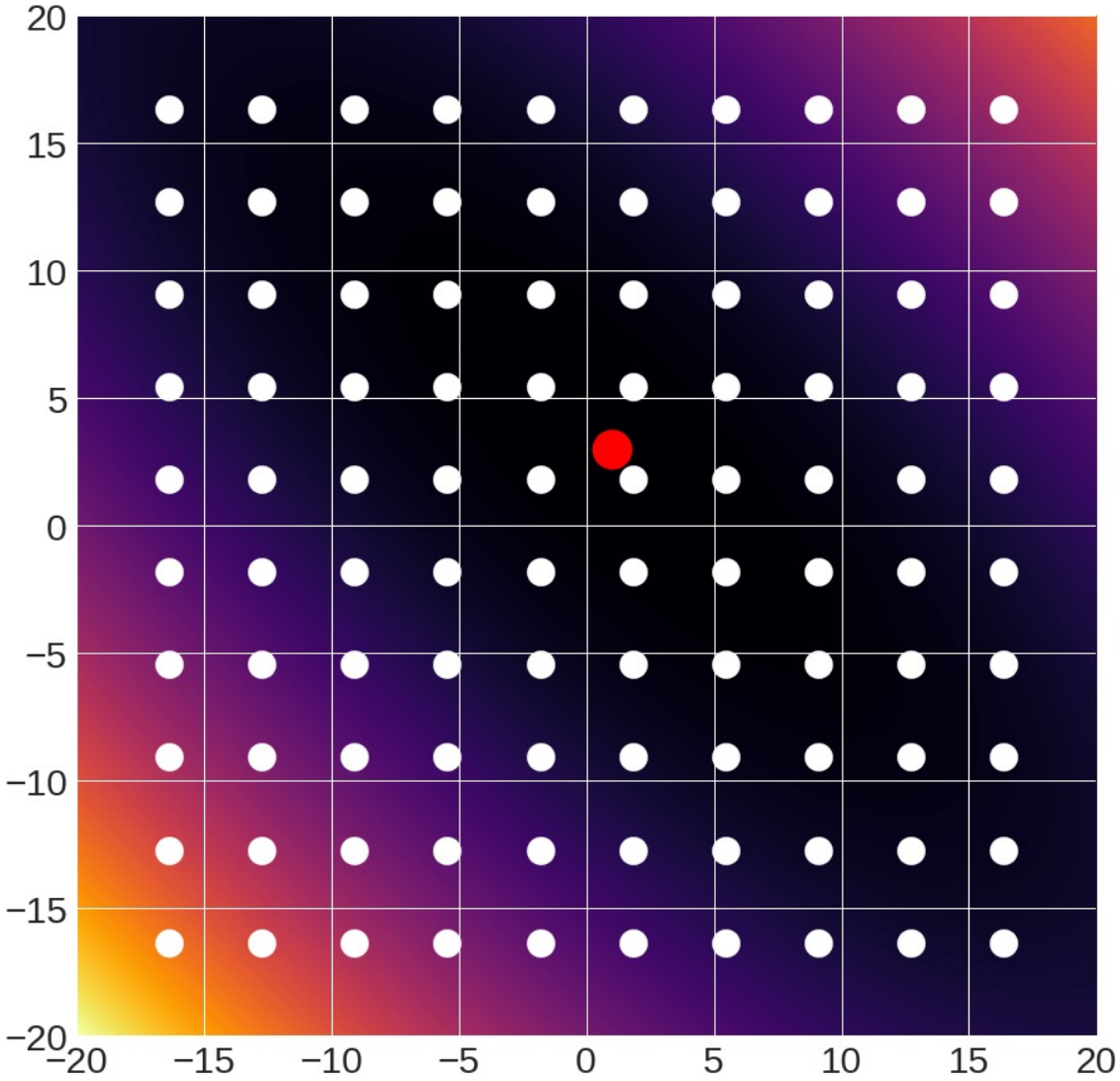
Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

Idea #1A: Grid Search

```
#systematically try things
best, bestScore = None, Inf
for dim1Value in dim1Values:
        ….
        for dimNValue in dimNValues:
                w = [dim1Value, …, dimNValue]
                if L(w) < bestScore:
                        best, bestScore = w, L(w)
return best
```

Slide credit: D Fouhey & J Johnson

Idea #1A: Grid Search



Slide credit: D Fouhey & J Johnson

Idea #1A: Grid Search

Pros:

1. Super simple
2. Only requires being able to evaluate model

Cons:

1. Scales horribly to high dimensional spaces

Complexity: $\text{samplesPerDim}^{\text{numberOfDims}}$

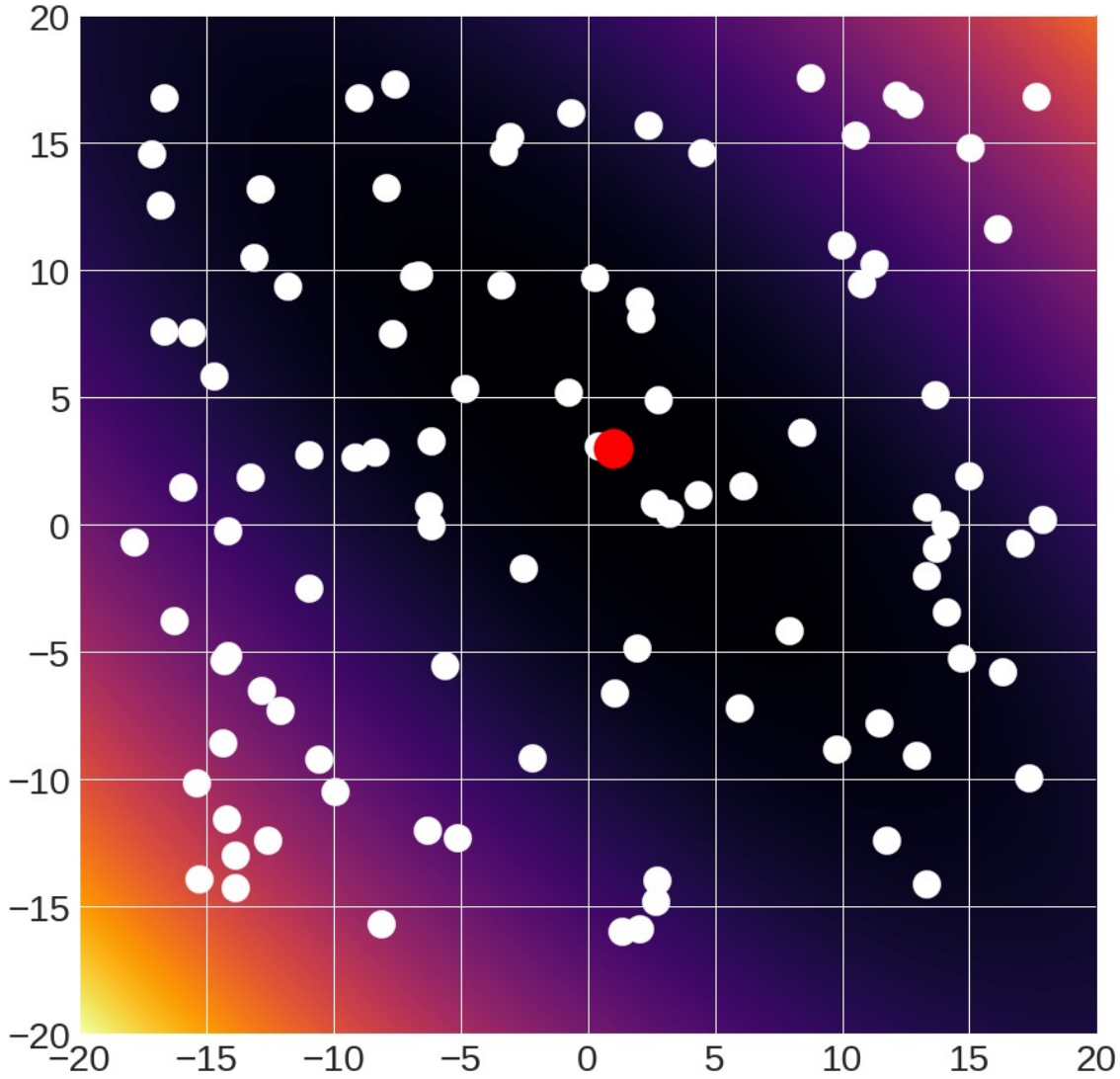
Slide credit: D Fouhey & J Johnson

Option #1B: Random Search

```
#Do random stuff RANSAC Style
best, bestScore = None, Inf
for iter in range(numIters):
        w = random(N,1) #sample
        score = L(w) #evaluate
        if score < bestScore:
                best, bestScore = w, score
return best
```

Slide credit: D Fouhey & J Johnson

Option #1B: Random Search



Slide credit: D Fouhey & J Johnson

Option #1B: Random Search

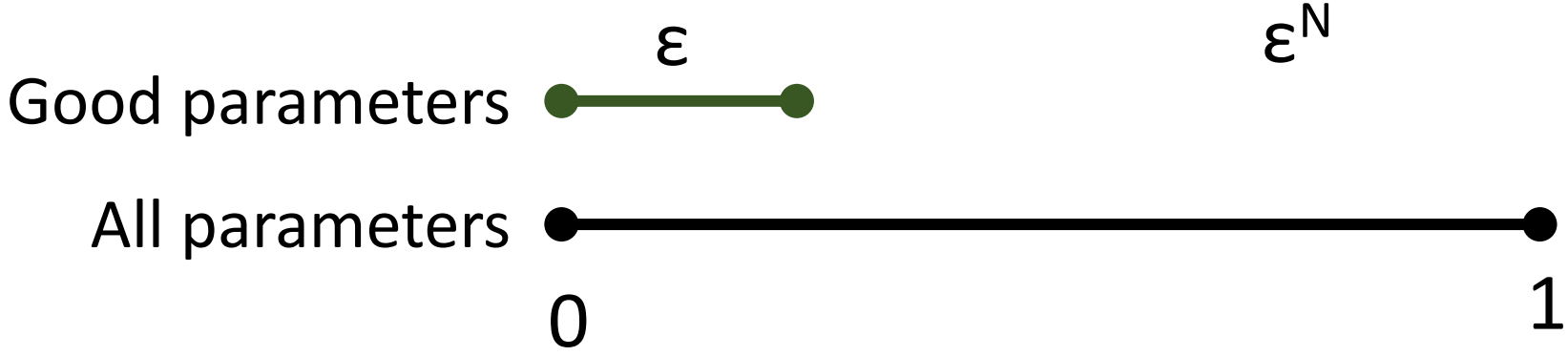
Pros:

1. Super simple
2. Only requires being able to sample model and evaluate it

Cons:

1. Slow –throwing darts at high dimensional dart board
2. Might miss something

P(all correct) = ε^N



Slide credit: D Fouhey & J Johnson

When To Use Options 1A / 1B?

Use these when

- Number of dimensions small, space bounded
- Objective is impossible to analyze

Random search is arguably more effective; grid search makes it easy to systematically test something (people love certainty)

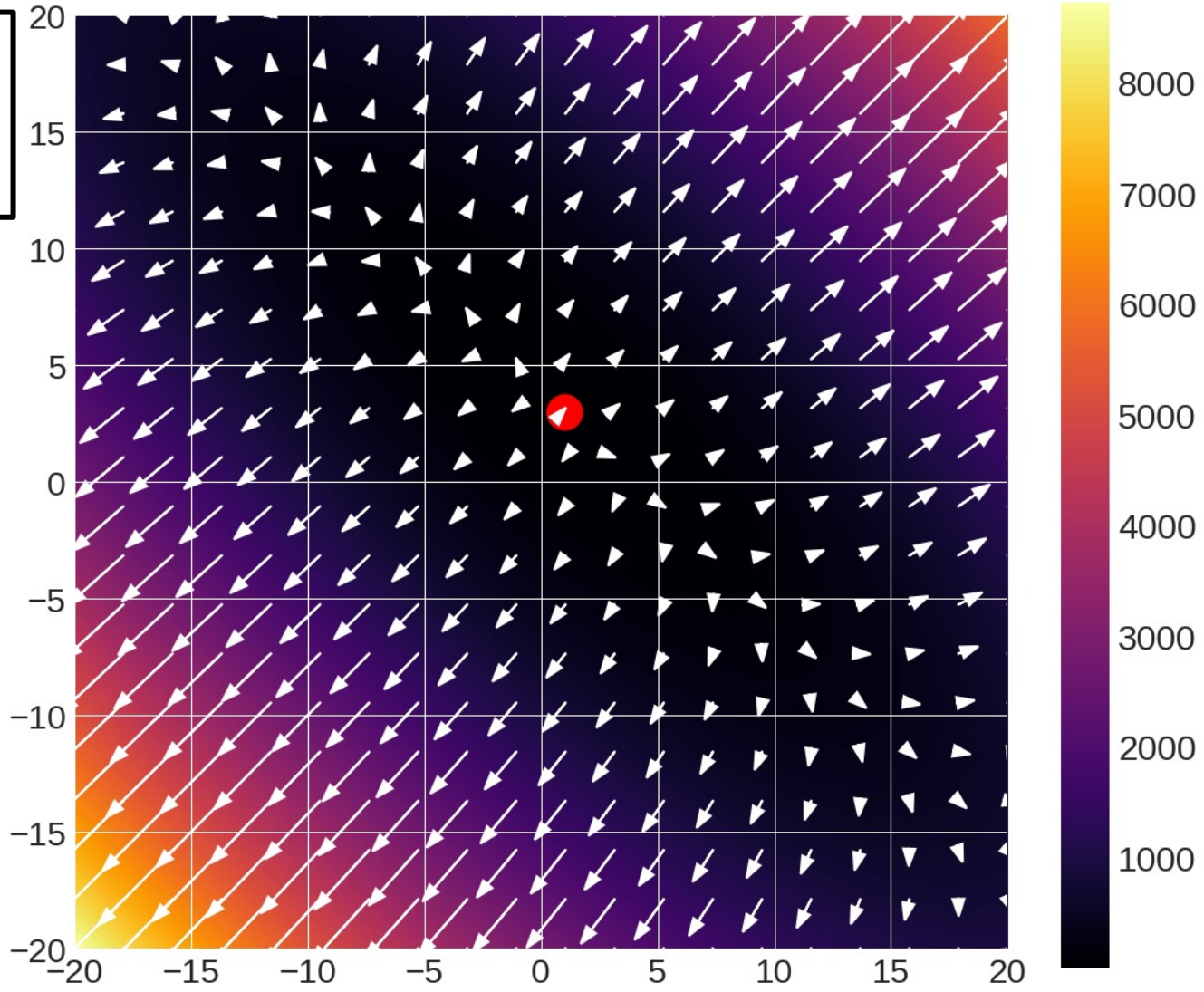
Slide credit: D Fouhey & J Johnson

Idea #2: Follow the slope

Slide credit: E Learned-Miller, originally developed by A Karpathy, J Johnson, Fei-Fei L

Idea #2: Follow the slope

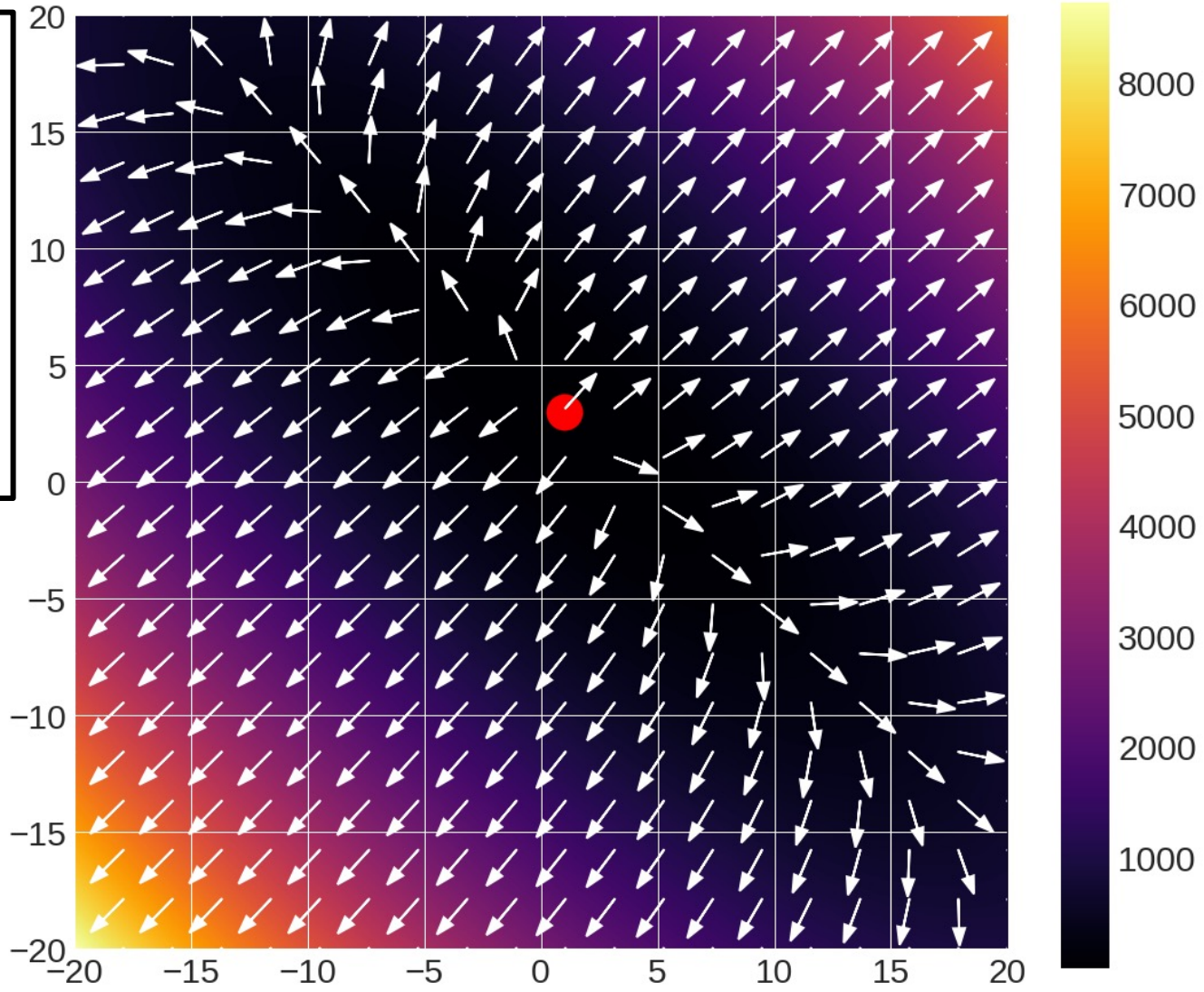
Arrows:
gradient



Slide credit: D Fouhey & J Johnson

Idea #2: Follow the slope

Arrows:
gradient direction
(scaled to unit length)



Slide credit: D Fouhey & J Johnson

Idea #2: Follow the slope

Want: $\arg\min_{\boldsymbol{w}} L(\boldsymbol{w})$

What's the geometric interpretation of: $\nabla_{\boldsymbol{w}} L(\boldsymbol{w}) = \begin{bmatrix} \partial L/\partial \boldsymbol{x}_1 \\ \vdots \\ \partial L/\partial \boldsymbol{x}_N \end{bmatrix}$

Which is bigger (for small α)?

$$L(\boldsymbol{w}) \quad \begin{matrix} \leq ? \\ > ? \end{matrix} \quad L(\boldsymbol{w} + \alpha \nabla_{\boldsymbol{w}} L(\boldsymbol{w}))$$

Slide credit: D Fouhey & J Johnson

Idea #2: Follow the slope

Method: at each step, move in direction of negative gradient

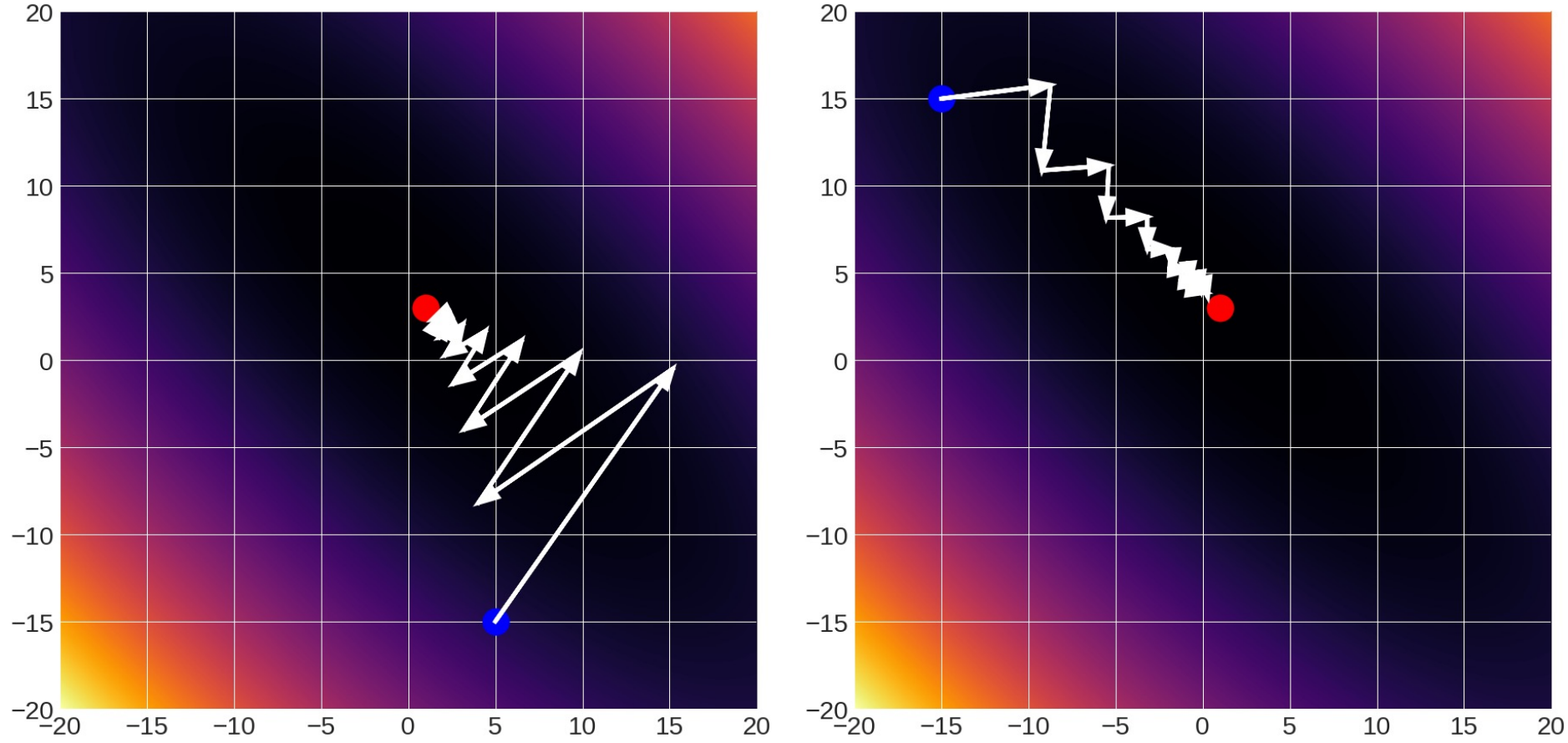
w0 = *initialize***()** #initialize
for iter in range(numIters):
    g = $\nabla_{\boldsymbol{w}} L(\boldsymbol{w})$ # eval gradient
    w = **w** + -*stepsize****g** # update w
return **w**

Slide credit: D Fouhey & J Johnson

Gradient Descent

Given starting point (blue)

$w_{i+1} = w_i + -9.8x10^{-2} * \text{gradient}$



Slide credit: D Fouhey & J Johnson

Computing Gradients: Numeric

How Do You Compute The Gradient?

Numerical Method:

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial L(w)}{\partial w_1} \\ \vdots \\ \frac{\partial L(w)}{\partial w_n} \end{bmatrix}$$

How do you compute this?

$$\frac{\partial f(x)}{\partial x} = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

In practice, use:

$$\frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}$$

Slide credit: D Fouhey & J Johnson

Computing Gradients: Numeric

How Do You Compute The Gradient?

Numerical Method:

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial L(w)}{\partial x_1} \\ \vdots \\ \frac{\partial L(w)}{\partial x_n} \end{bmatrix}$$

Use: $\frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}$

How many function evaluations per dimension?

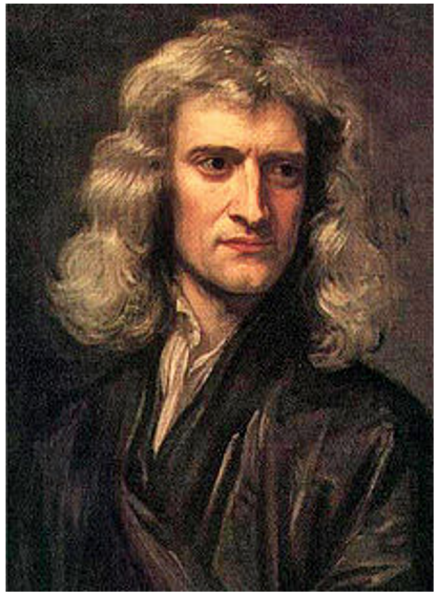
Slide credit: D Fouhey & J Johnson

Computing Gradients: Analytic

How Do You Compute The Gradient?

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial L(w)}{\partial x_1} \\ \vdots \\ \frac{\partial L(w)}{\partial x_n} \end{bmatrix}$$

Better Idea: Use Calculus!



This image is in the public domain

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Slide credit: D Fouhey & J Johnson

Retropolis

During a pandemic, Isaac Newton had to work from home, too. He used the time wisely.

A later portrait of Sir Isaac Newton by Samuel Freeman. (British Library/National Endowment for the Humanities)

By **Gillian Brockell**

March 12, 2020 at 2:18 p.m. EDT

Isaac Newton was in his early 20s when the Great Plague of London hit. He wasn't a "Sir" yet, didn't

1. Developed calculus
2. Fundamentals of optics
3. Theory of gravity

Slide credit: E Learned-Miller

Computing Gradients

- **Numeric gradient**: approximate, slow, easy to write
- **Analytic gradient**: exact, fast, error-prone

In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check.**

`torch.autograd.gradcheck(`*`func`*`,` *`inputs`*`,` *`eps=1e-06`*`,` *`atol=1e-05`*`,` *`rtol=0.001`*`,` *`raise_exception=True`*`,` *`check_sparse_nnz=False`*`,` *`nondet_tol=0.0`*`)` [SOURCE]

Check gradients computed via small finite differences against analytical gradients w.r.t. tensors in `inputs` that are of floating point type and with `requires_grad=True`.

The check between numerical and analytical gradients uses `allclose()`.

Slide credit: D Fouhey & J Johnson

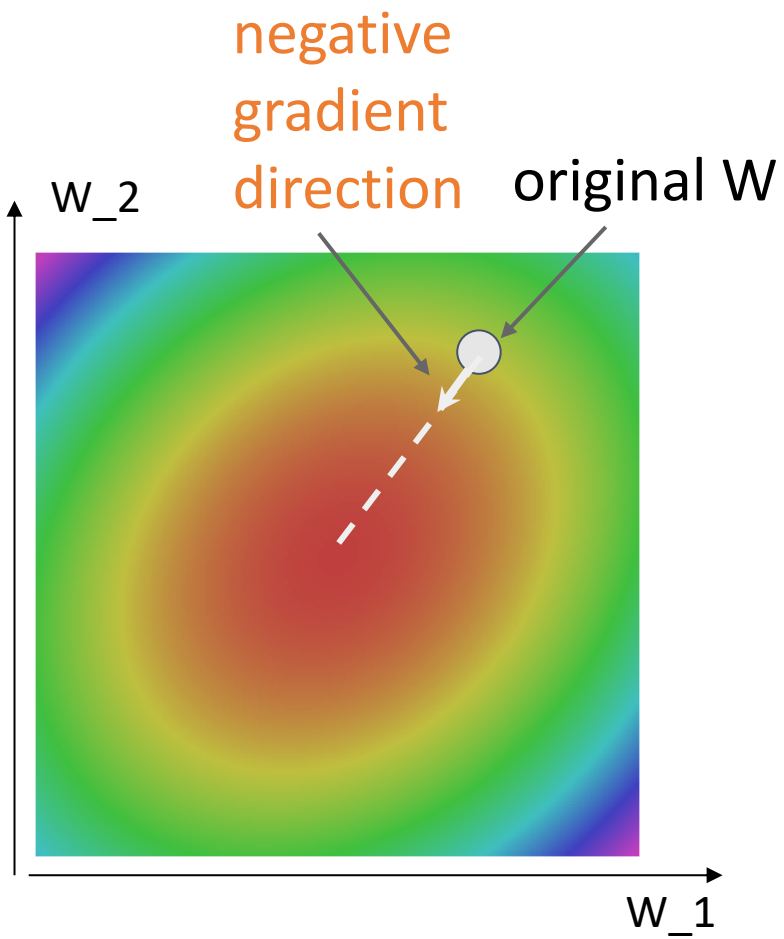
Gradient Descent

Iteratively step in the direction of the negative gradient
(direction of local steepest descent)

```
# Vanilla gradient descent
w = initialize_weights()
for t in range(num_steps):
  dw = compute_gradient(loss_fn, data, w)
  w -= learning_rate * dw
```

Hyperparameters:

- Weight initialization method
- Number of steps
- Learning rate



Slide credit: D Fouhey & J Johnson

Batch Gradient Descent

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Problem: Full sum is expensive when N is large!

$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Solution: Approximate sum using a **minibatch** of examples, e.g. 32

Slide credit: D Fouhey & J Johnson

Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Problem: Full sum is expensive when N is large!

$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Solution: Approximate sum using a **minibatch** of examples, e.g. 32

```
# Stochastic gradient descent
w = initialize_weights()
for t in range(num_steps):
  minibatch = sample_data(data, batch_size)
  dw = compute_gradient(loss_fn, minibatch, w)
  w -= learning_rate * dw
```

Hyperparameters:

- Weight initialization
- Number of steps
- Learning rate
- Batch size
- Data sampling

Slide credit: D Fouhey & J Johnson

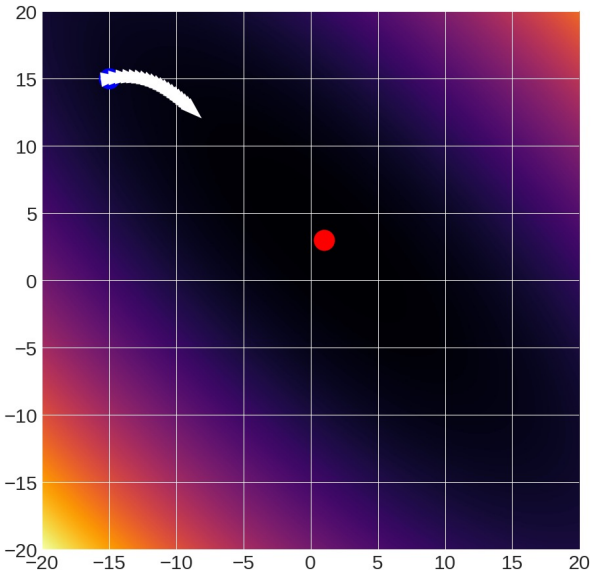
Gradient Descent: Learning Rate

Step size (also called **learning rate / lr**)

critical parameter

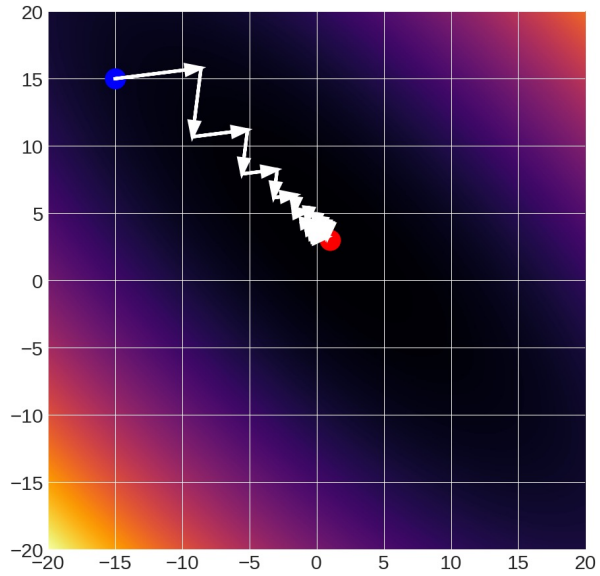
$1x10^{-2}$

falls short



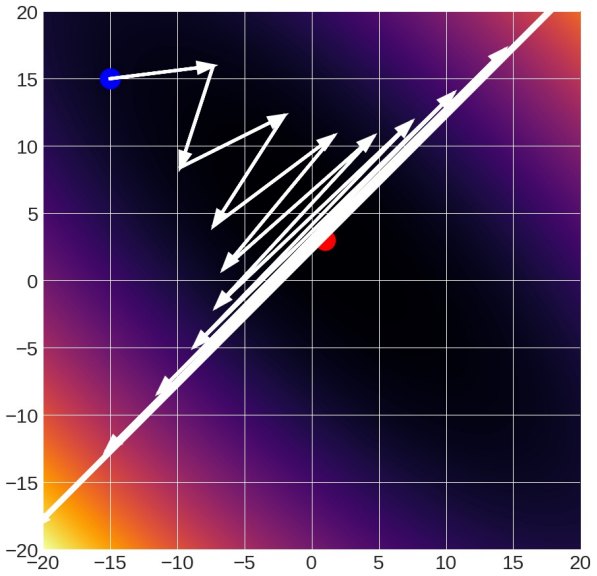
$10x10^{-2}$

converges



$12x10^{-2}$

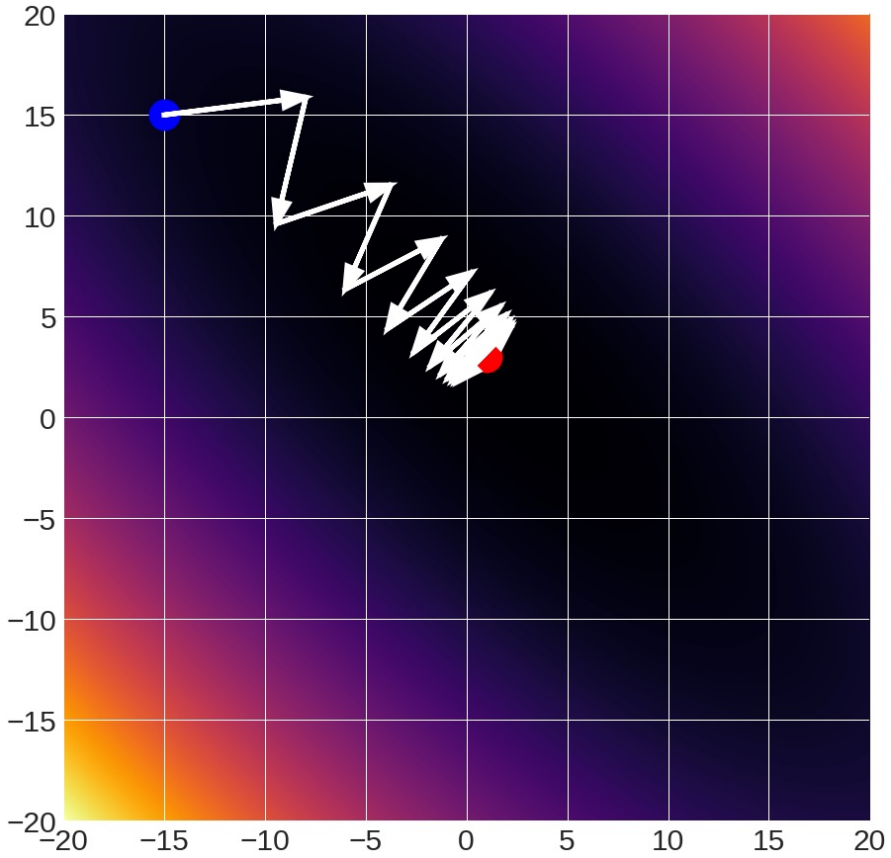
diverges



Slide credit: D Fouhey & J Johnson

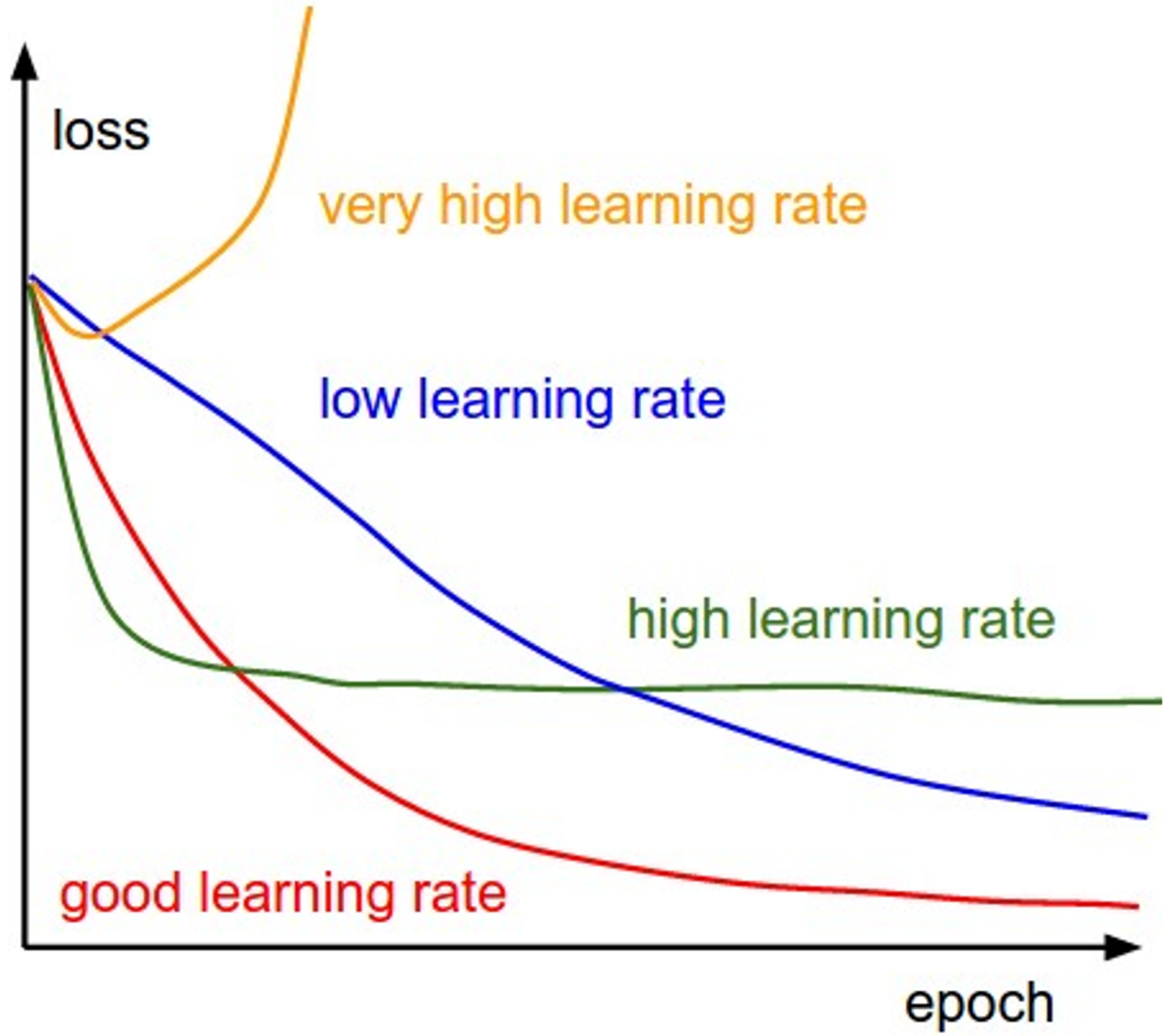
Gradient Descent: Learning Rate

$11x10^{-2}$:oscillates



Slide credit: D Fouhey & J Johnson

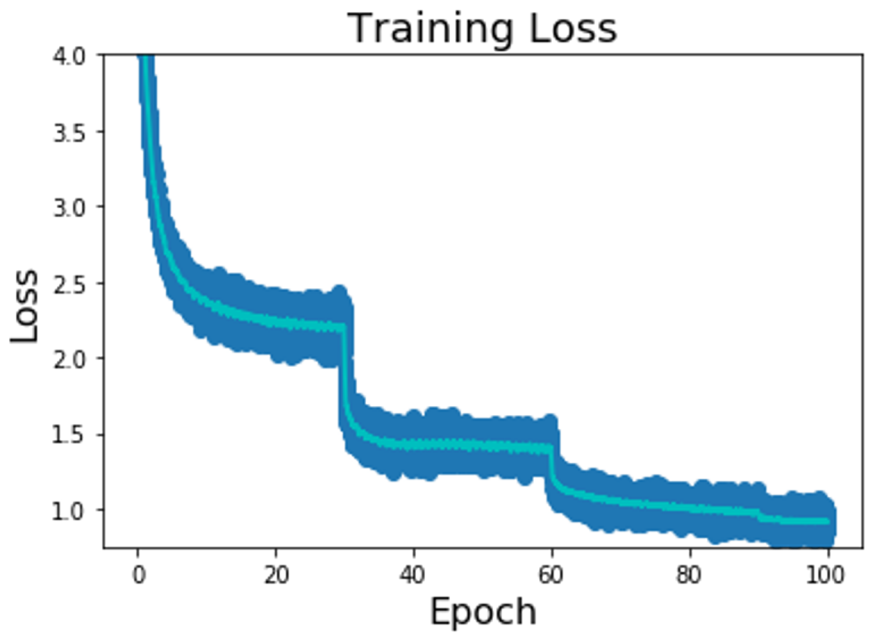
Effects of Learning Rate (Step Size)

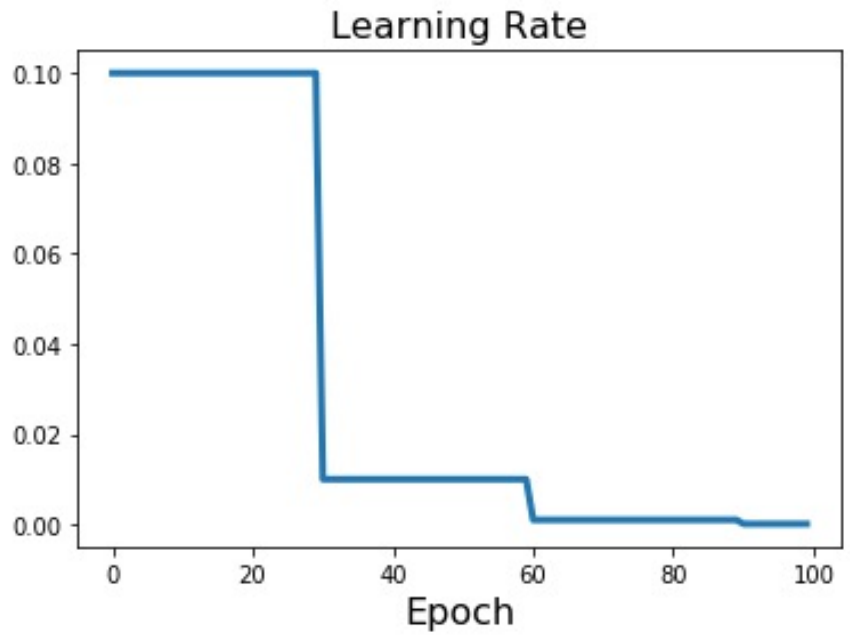


Slide credit: E Learned-Miller

Learning Rate Decay

Idea: Start with high learning rate, reduce it over time.
Step Decay: Reduce by some factor at fixed iterations



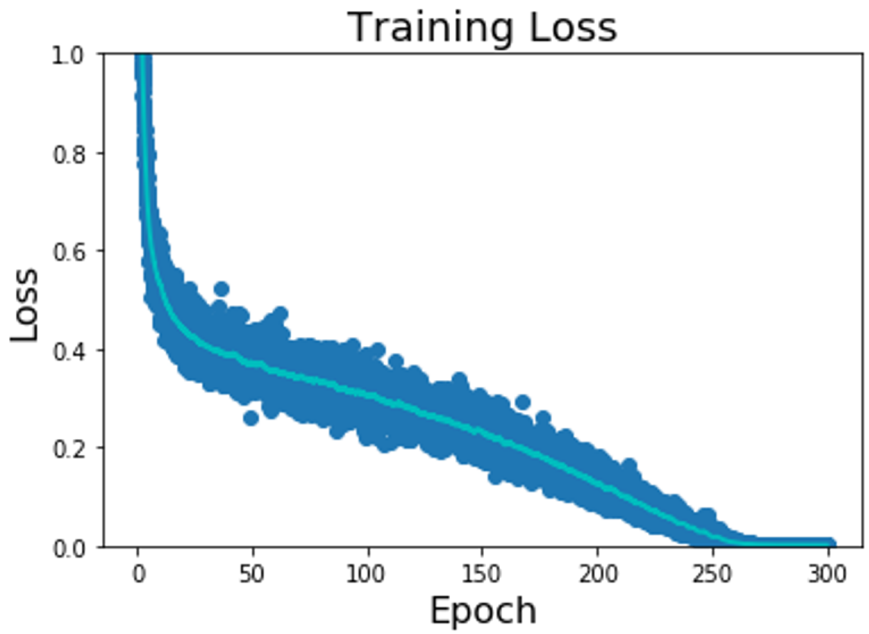


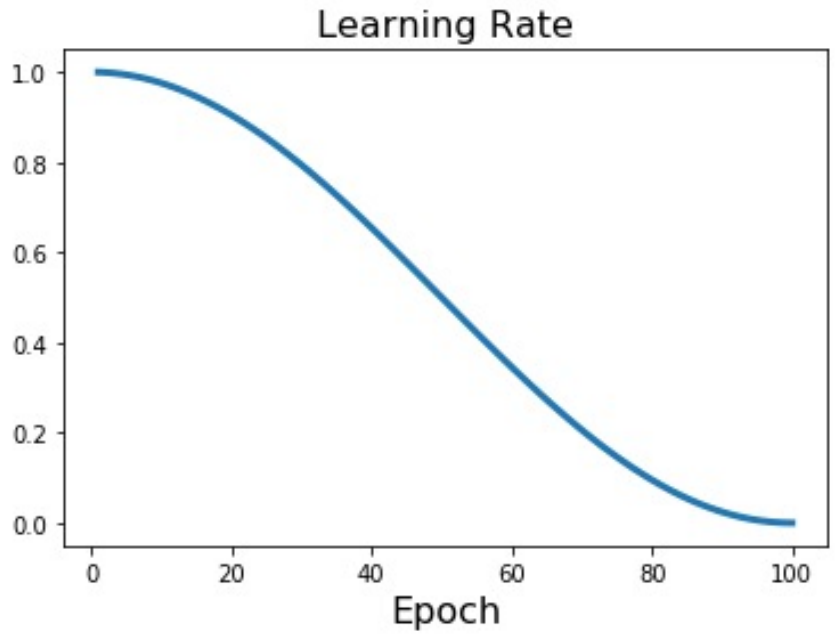
Slide credit: D Fouhey & J Johnson

Learning Rate Decay

Idea: Start with high learning rate, reduce it over time.

Cosine Decay: $\alpha_t = \frac{1}{2}\alpha_0\left(1 + cos\left(\frac{t\pi}{T}\right)\right)$

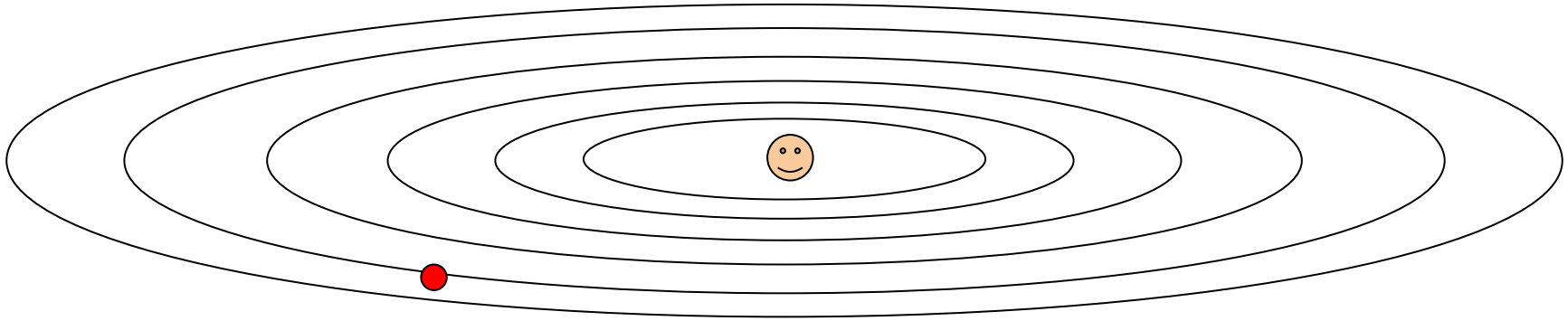




Slide credit: D Fouhey & J Johnson

Problems with SGD

What if loss changes quickly in one direction and slowly in another?

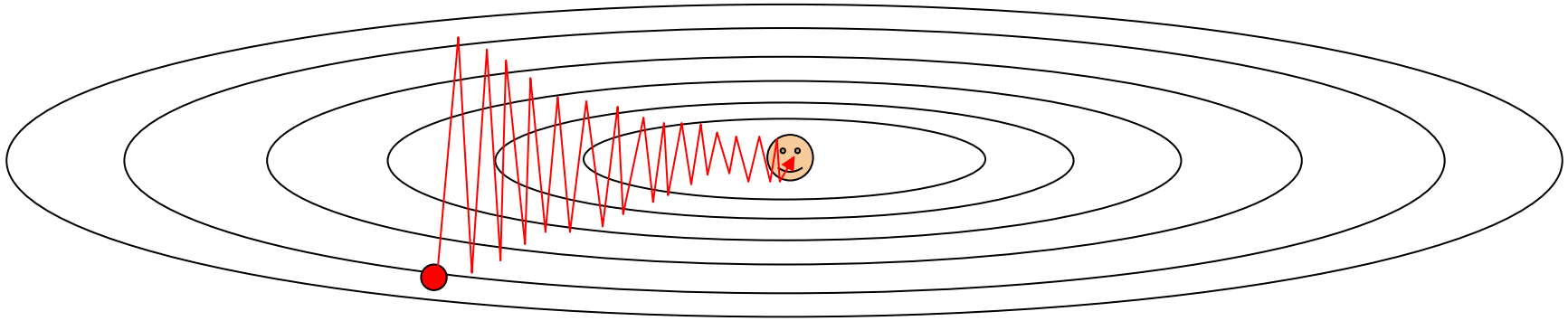


Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Slide credit: D Fouhey & J Johnson

Problems with SGD

What if loss changes quickly in one direction and slowly in another?
Slow progress along shallow dimension, jitter along steep direction



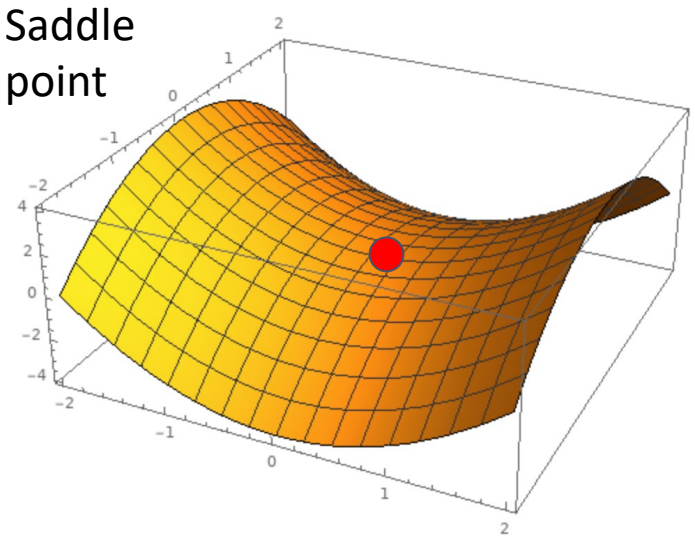
Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Slide credit: D Fouhey & J Johnson

Problems with SGD

What if the loss function has a **local minimum** or **saddle point**?

Gradient is zero,
SGD gets stuck



Slide credit: D Fouhey & J Johnson

Problems with SGD

Our gradients come from minibatches so they can be noisy!

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Slide credit: D Fouhey & J Johnson

SGD

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Slide credit: D Fouhey & J Johnson

SGD + Momentum

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD + Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically $\rho = 0.9$ or 0.99

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Slide credit: D Fouhey & J Johnson

SGD + Momentum

SGD + Momentum

$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v - learning_rate * dw
  w += v
```

SGD + Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

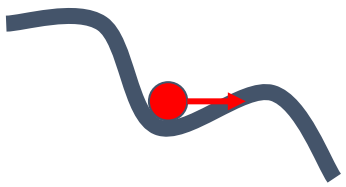
You may see SGD+Momentum formulated different ways, but they are equivalent - give same sequence of x

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

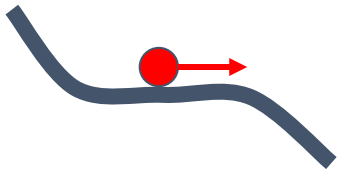
Slide credit: D Fouhey & J Johnson

SGD + Momentum

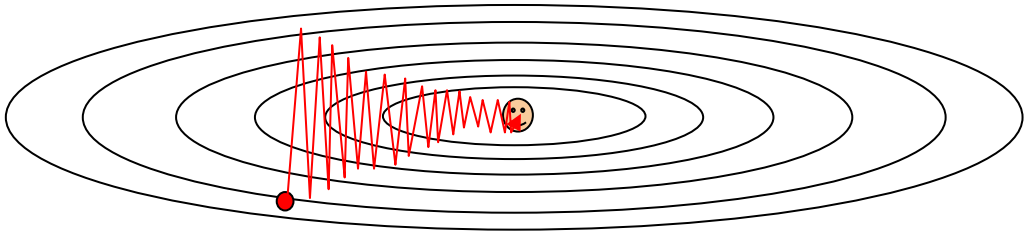
Local Minima



Saddle points



Poor Conditioning



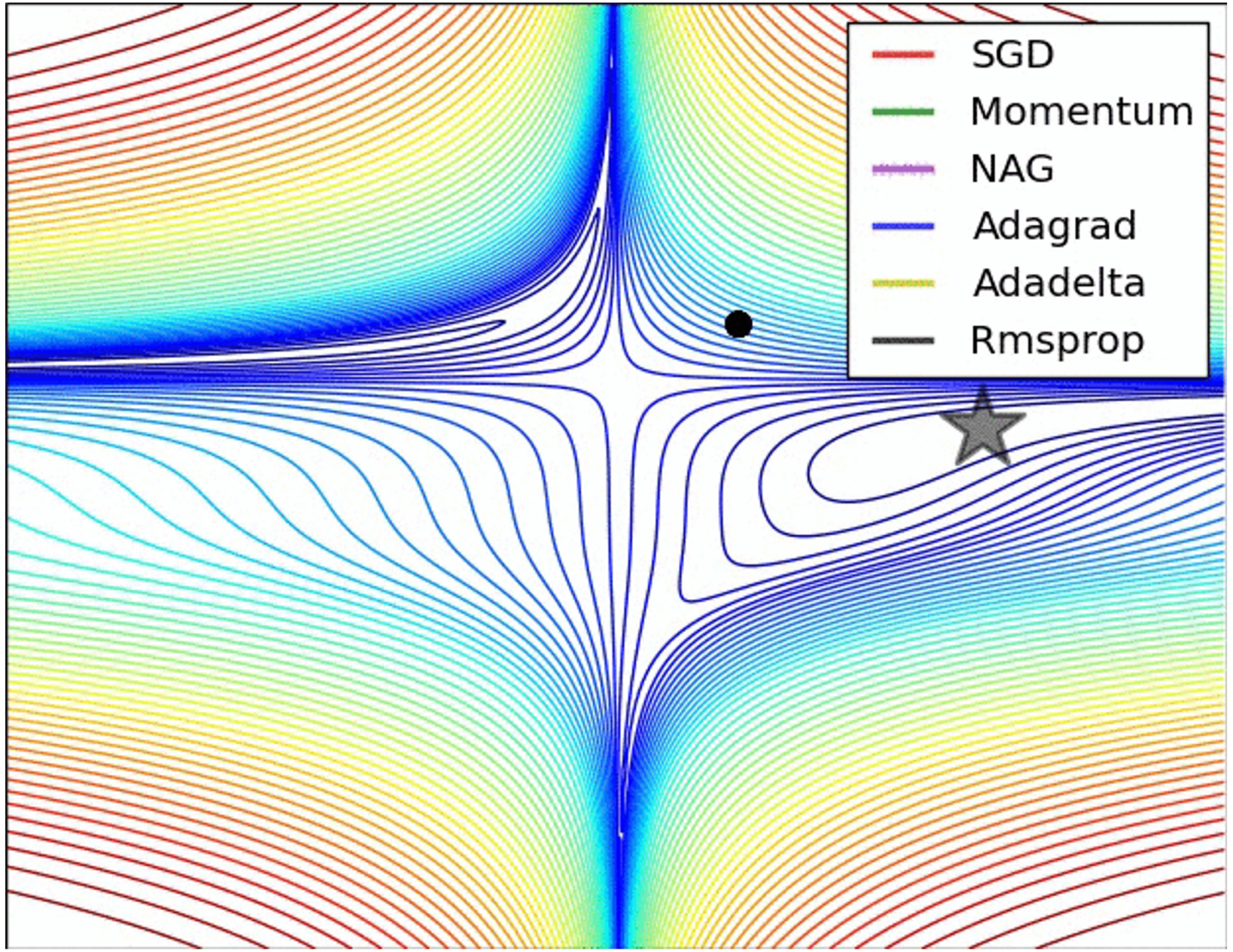
Gradient Noise

SGD SGD+Momentum

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Slide credit: D Fouhey & J Johnson

The effects of different update form formulas



(image credits to Alec Radford)

Slide credit: E Learned-Miller

Optimization in Practice

- **Conventional wisdom**: minibatch stochastic gradient descent (SGD) + momentum (package implements it for you) + some sensibly changing learning rate
- The above is typically what is meant by “SGD”
- Other update rules exist (Adam very common); sometimes better, sometimes worse than SGD

Slide credit: D Fouhey & J Johnson

Optimizing Everything

$$L(\boldsymbol{W}) = \boldsymbol{\lambda}\|\boldsymbol{W}\|_{\boldsymbol{2}}^{\boldsymbol{2}} + \sum_{i=1}^{n} -\log\left(\frac{\exp((Wx)_{y_i})}{\sum_k \exp((Wx)_k))}\right)$$

$$L(\boldsymbol{w}) = \lambda\|\boldsymbol{w}\|_2^2 + \sum_{i=1}^{n}\left(y_i - \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}_{\boldsymbol{i}}\right)^2$$

- Optimize **w** on training set with SGD to maximize training accuracy
- Optimize λ with random/grid search to maximize validation accuracy
- Note: Optimizing λ on training sets it to 0

Slide credit: D Fouhey & J Johnson

Next Class

Neural Networks!