Optimization: Stochastic Gradient Descent

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Gradient Descent

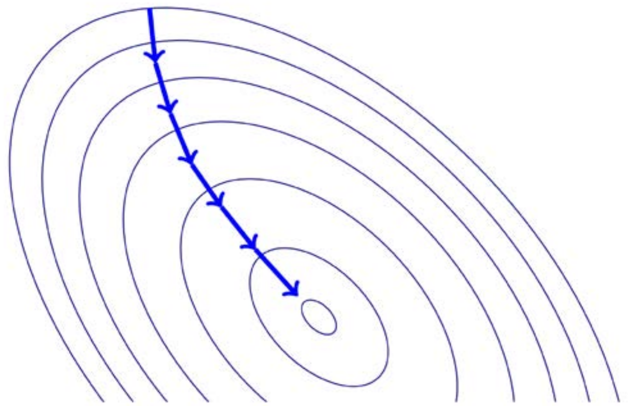
- We will cover gradient descent algorithm and its variants:
  - Batch Gradient Descent
  - Stochastic Gradient Descent
  - Mini-batch Gradient Descent

- We will explore the concept of these three gradient descent algorithms with a logistic regression model in TensorFlow

- Limitation of the Gradient Descent
  - Adaptive learning rate

Batch Gradient Descent (= Gradient Descent)

Repeat: $\omega \leftarrow \omega - \alpha \nabla f(\omega)$ for some step size (or learning rate) $\alpha > 0$



Batch Gradient Descent

- Loss function ℓ has been the average loss over all of the training examples:

$$\mathcal{E}(\omega) = \frac{1}{m}\sum_{i=1}^{m}\ell(\hat{y}_i, y_i) = \frac{1}{m}\sum_{i=1}^{m}\ell(h_\omega(x_i), y_i)$$

- By linearity,

$$\nabla_\omega \mathcal{E} = \nabla_\omega \frac{1}{m}\sum_{i=1}^{m}\ell(h_\omega(x_i), y_i) = \frac{1}{m}\sum_{i=1}^{m}\frac{\partial}{\partial\omega}\ell(h_\omega(x_i), y_i)$$

$$\omega \leftarrow \omega - \alpha\,\nabla_\omega \mathcal{E}$$

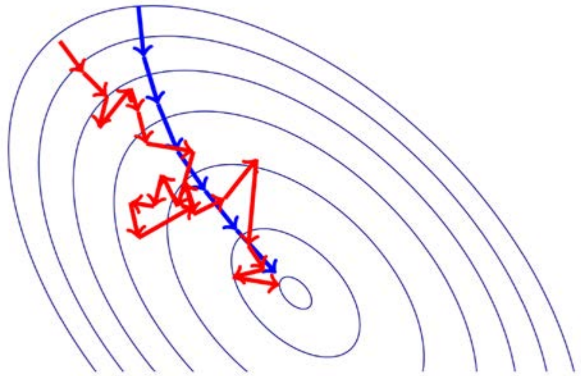
- Computing the gradient requires summing over all of the training examples.
- This is known as batch training.
- Batch training is impractical if you have a large dataset (e.g. millions of training examples) !

Stochastic Gradient Descent (SGD)

- Stochastic gradient descent (SGD): update the parameters based on the gradient for a randomly selected single training example:

$$\ell(\hat{y}_i, y_i) = \ell(h_\omega(x_i), y_i) = \ell^{(i)}$$

$$\omega \leftarrow \omega - \alpha \frac{\partial \ell^{(i)}}{\partial \omega}$$

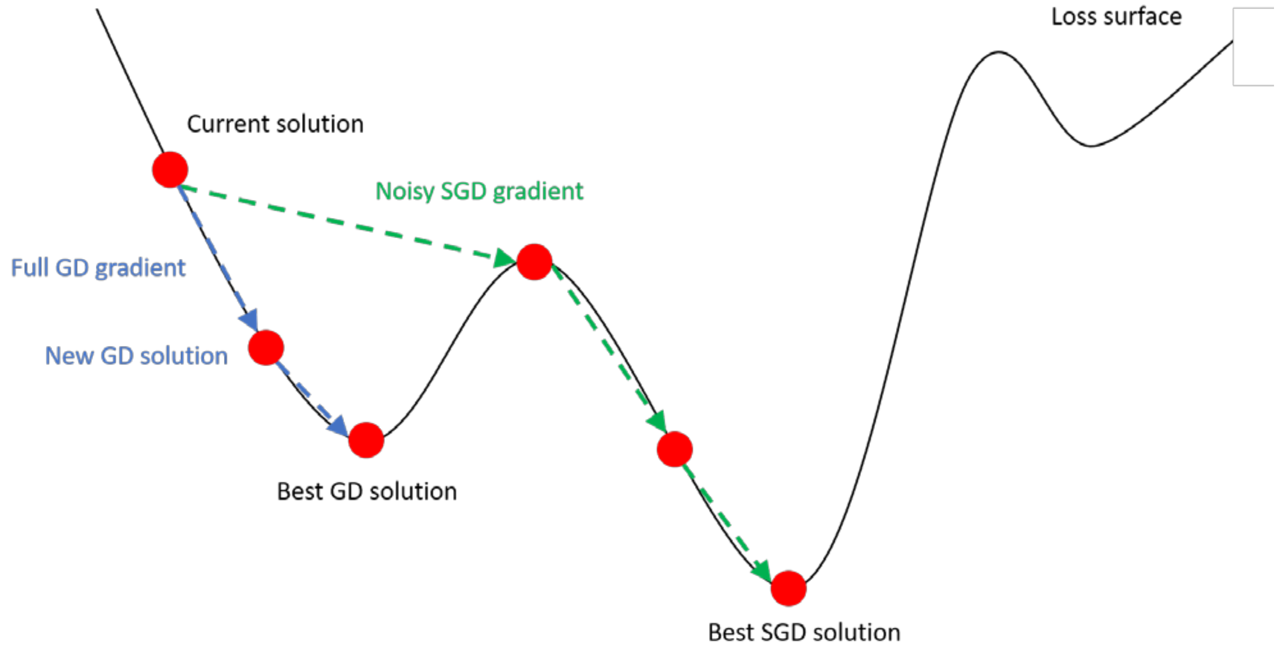


  - SGD takes steps in a noisy direction, but moves downhill on average.

- Mathematical justification: if you sample a training example at random, the stochastic gradient is an unbiased estimate of the batch gradient:

$$\mathbb{E}\left[\frac{\partial \ell^{(i)}}{\partial \omega}\right] = \frac{1}{m}\sum_{i=1}^{m}\frac{\partial \ell^{(i)}}{\partial \omega} = \frac{\partial}{\partial \omega}\left[\frac{1}{m}\sum_{i=1}^{m}\ell^{(i)}\right] = \frac{\partial \mathcal{E}}{\partial \omega}$$

SGD is Sometimes Better



- No guarantee that this is what is going to always happen.
- But the noisy SGD gradients can help occasionally escaping local optima

Mini-batch Gradient Descent

- Potential problem of SGD: gradient estimates can be very noisy

- Compromise approach: compute the gradients on a medium-sized set of training examples s $(< m)$, called a mini-batch.

$$\mathcal{E}(\omega) = \frac{1}{s}\sum_{i=1}^{s} \ell(\hat{y}_i, y_i) = \frac{1}{s}\sum_{i=1}^{s} \ell(h_\omega(x_i), y_i) = \frac{1}{s}\sum_{i=1}^{s} \ell^{(i)}$$

$$\omega \leftarrow \omega - \alpha \nabla_\omega \mathcal{E}$$

- Stochastic gradients computed on larger mini-batches have smaller variance:

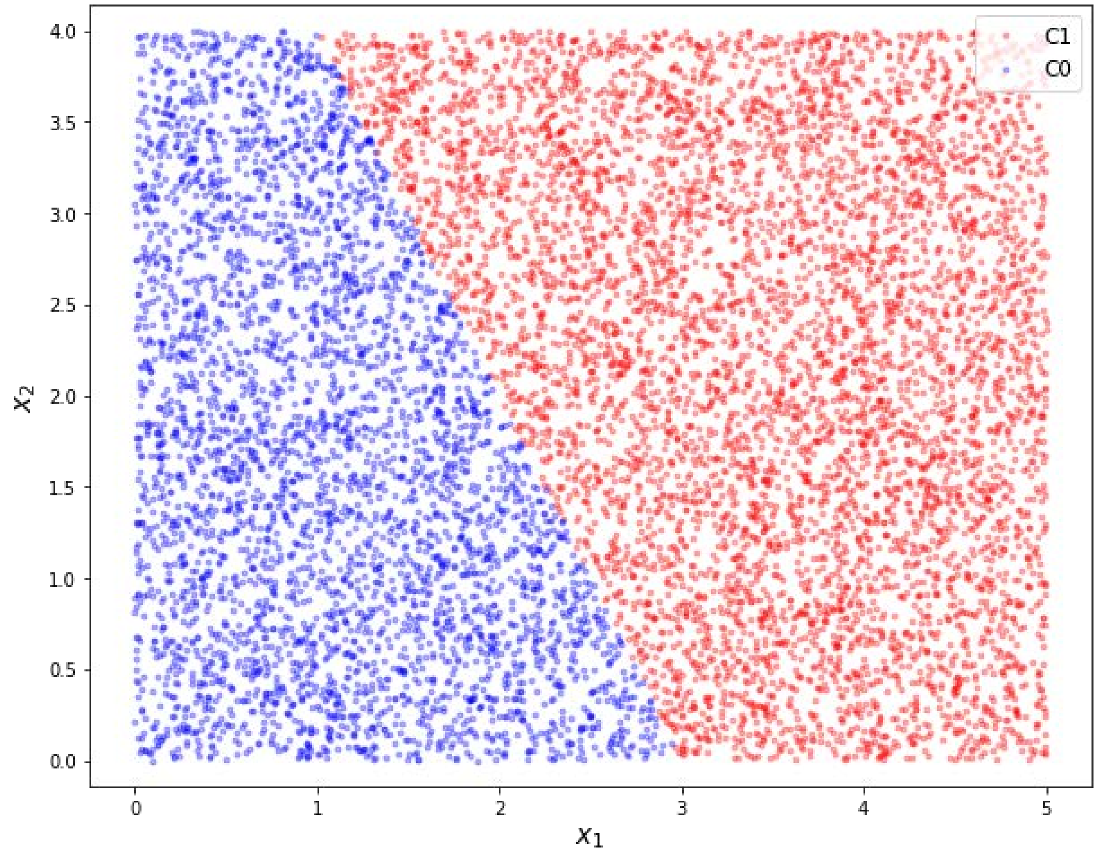
$$\text{var}\left[\frac{1}{s}\sum_{i=1}^{s}\frac{\partial \ell^{(i)}}{\partial \omega}\right] = \frac{1}{s^2}\text{var}\left[\sum_{i=1}^{s}\frac{\partial \ell^{(i)}}{\partial \omega}\right] = \frac{1}{s}\text{var}\left[\frac{\partial \ell^{(i)}}{\partial \omega}\right]$$

- The mini-batch size s is a hyper-parameter that needs to be set.

Implementation with TensorFlow

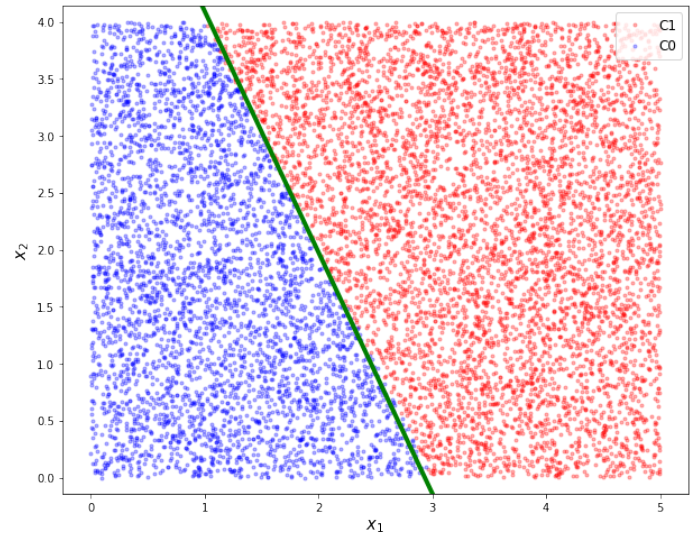
Batch Gradient Descent with TensorFlow

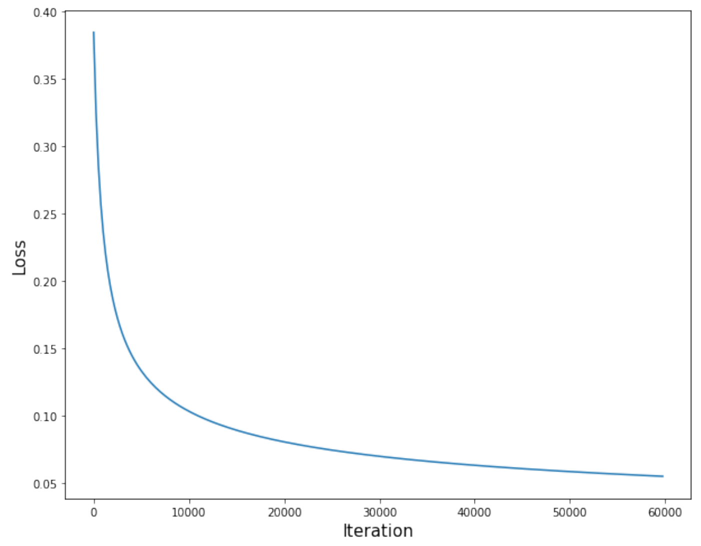
- We will explore the python codes of these three gradient descent algorithms with a logistic regression model.



Batch Gradient Descent with TensorFlow

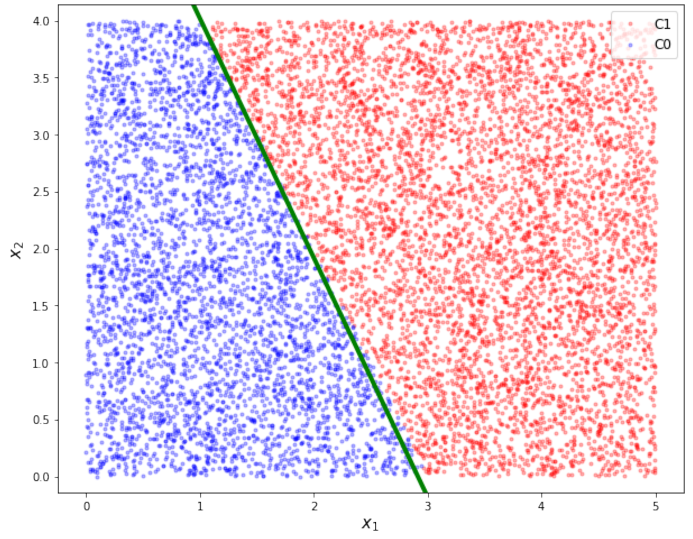
```python
LR = 0.04
n_iter = 60000
n_prt = 250

x = tf.placeholder(tf.float32, [m, 3])
y = tf.placeholder(tf.float32, [m, 1])

w = tf.Variable([[0],[0],[0]], dtype = tf.float32)

y_pred = tf.matmul(x,w)
loss = tf.nn.sigmoid_cross_entropy_with_logits(logits=y_pred, labels=y)
loss = tf.reduce_mean(loss)

optm = tf.train.GradientDescentOptimizer(LR).minimize(loss)
init = tf.global_variables_initializer()

start_time = time.time()

loss_record = []
with tf.Session() as sess:
    sess.run(init)
    for epoch in range(n_iter):
        sess.run(optm, feed_dict = {x: train_X, y: train_y})

        if (epoch + 1) % n_prt == 0:
            loss_record.append(sess.run(loss, feed_dict = {x: train_X, y: train_y}))

    w_hat = sess.run(w)
```

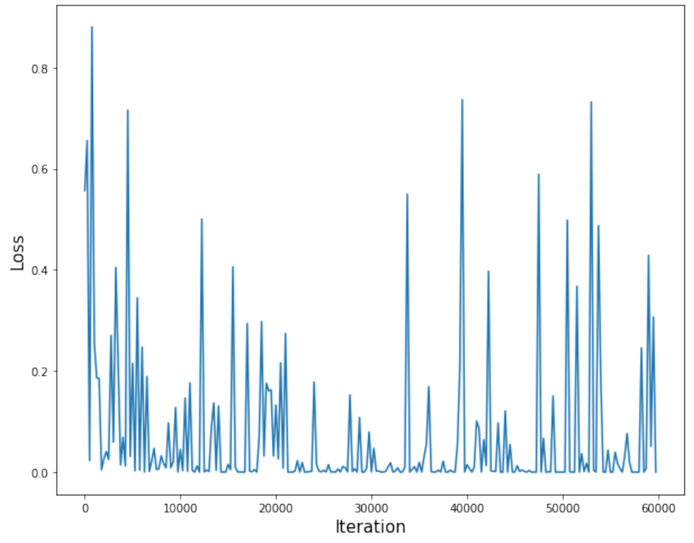




Stochastic Gradient Descent (SGD) with TensorFlow

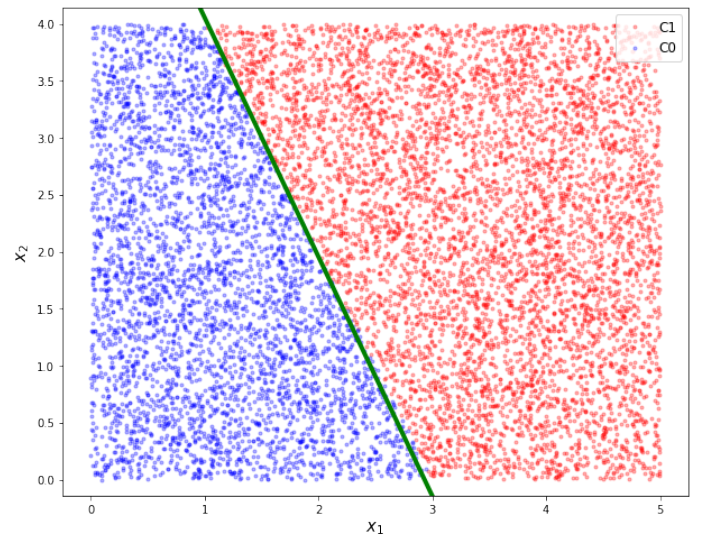
```
LR = 0.04
n_iter = 60000
n_prt = 250

x = tf.placeholder(tf.float32, [1, 3])
y = tf.placeholder(tf.float32, [1, 1])

w = tf.Variable(tf.random_normal([3,1]), dtype = tf.float32)

y_pred = tf.matmul(x,w)
loss = tf.nn.sigmoid_cross_entropy_with_logits(logits=y_pred, labels=y)
loss = tf.reduce_mean(loss)

optm = tf.train.GradientDescentOptimizer(LR).minimize(loss)
init = tf.global_variables_initializer()

start_time = time.time()

loss_record = []
with tf.Session() as sess:
    sess.run(init)
    for epoch in range(n_iter):
        idx = np.random.choice(m, 1)
        batch_X = train_X[idx,:]
        batch_y = train_y[idx]
        sess.run(optm, feed_dict = {x: batch_X, y: batch_y})

        if (epoch + 1) % n_prt == 0:
            loss_record.append(sess.run(loss, feed_dict = {x: batch_X, y: batch_y}))

    w_hat = sess.run(w)
```

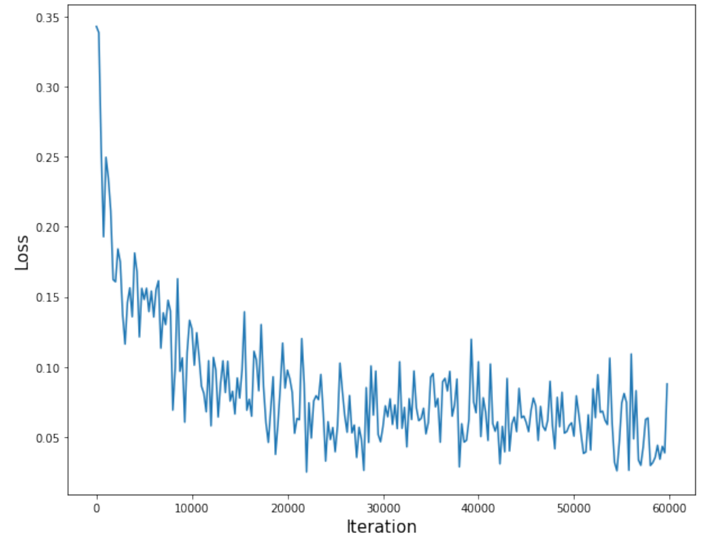




Mini-batch Gradient Descent with TensorFlow

```
LR = 0.04
n_iter = 60000
n_batch = 50
n_prt = 250

x = tf.placeholder(tf.float32, [n_batch, 3])
y = tf.placeholder(tf.float32, [n_batch, 1])

w = tf.Variable(tf.random_normal([3,1]), dtype = tf.float32)

y_pred = tf.matmul(x,w)
loss = tf.nn.sigmoid_cross_entropy_with_logits(logits=y_pred, labels=y)
loss = tf.reduce_mean(loss)

optm = tf.train.GradientDescentOptimizer(LR).minimize(loss)
init = tf.global_variables_initializer()

start_time = time.time()

loss_record = []
with tf.Session() as sess:
    sess.run(init)
    for epoch in range(n_iter):
        idx = np.random.choice(m, size = n_batch)
        batch_X = train_X[idx,:]
        batch_y = train_y[idx]
        sess.run(optm, feed_dict = {x: batch_X, y: batch_y})

        if (epoch + 1) % n_prt == 0:
            loss_record.append(sess.run(loss, feed_dict = {x: batch_X, y: batch_y}))

    w_hat = sess.run(w)
```





POSTECH

Limitation of the Gradient Descent

Setting the Learning Rate

- How can we set the learning rate?

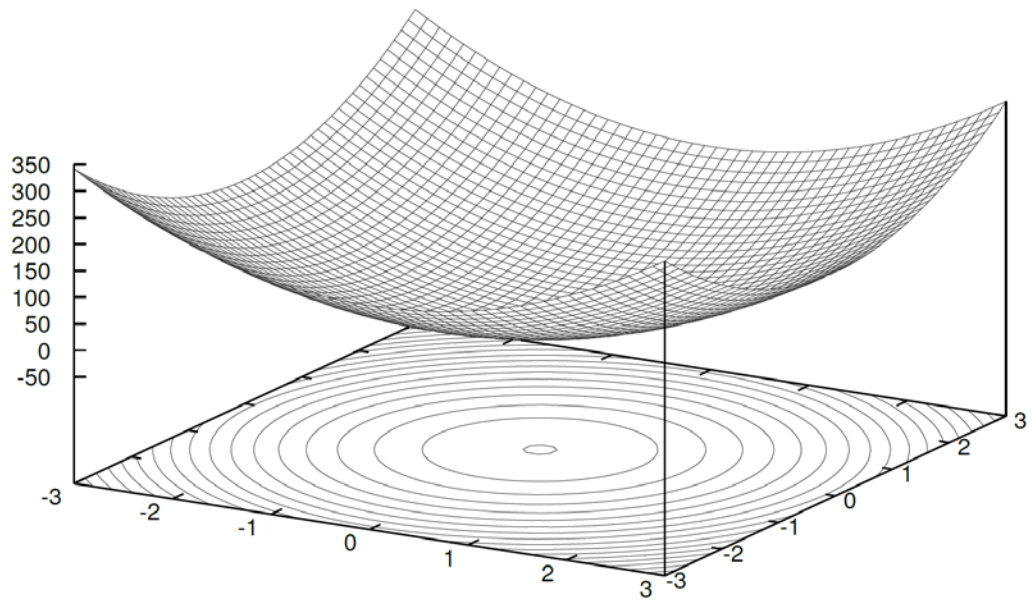
$$\omega_{k+1} = \omega_k - \underset{\uparrow}{\alpha} \nabla f(\omega_k)$$

- Small learning rate converges slowly and gets stuck in false local minima
- Large learning rates overshoot, become unstable and diverge

- Idea 1
  - Try lots of different learning rates and see what works "just right"
- Idea 2
  - Do something smarter! Design an adaptive learning rate that "adapts" to the landscape
  - Temporal and spatial

SGD Learning Rate (= Step Size)

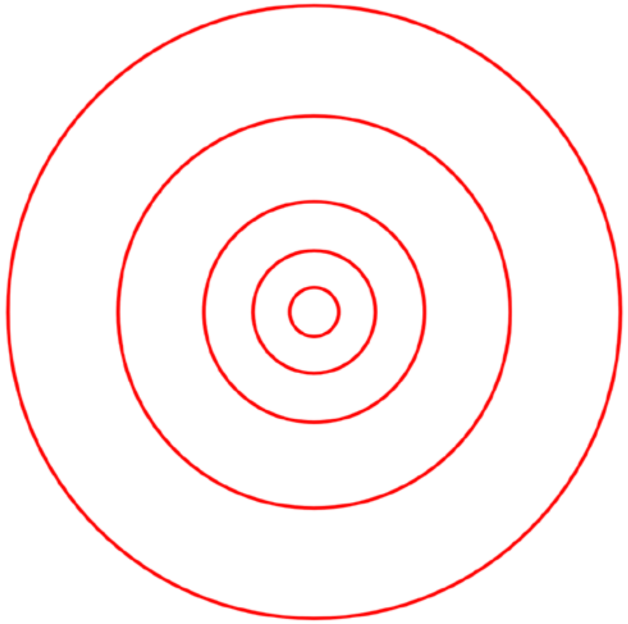
- The gradient descent method makes a strong assumption about the magnitude of the “local curvature” to fix the step size, and about its isotropy so that the same step size makes sense in all directions.



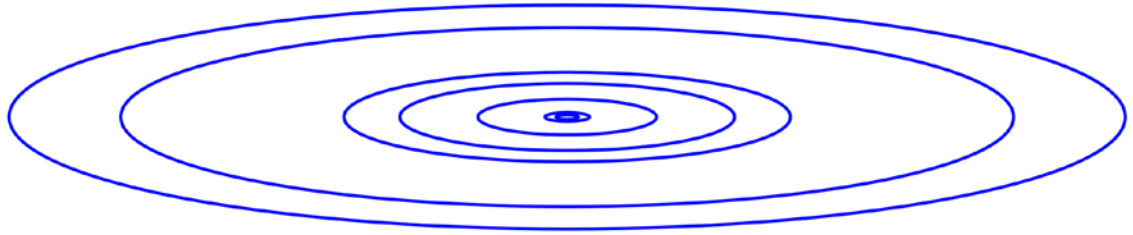
Source: Dr. Francois Fleuret at EPFL

SGD Learning Rate: Spatial

- We assign the same learning rate to all features



Nice (all features are equally important)



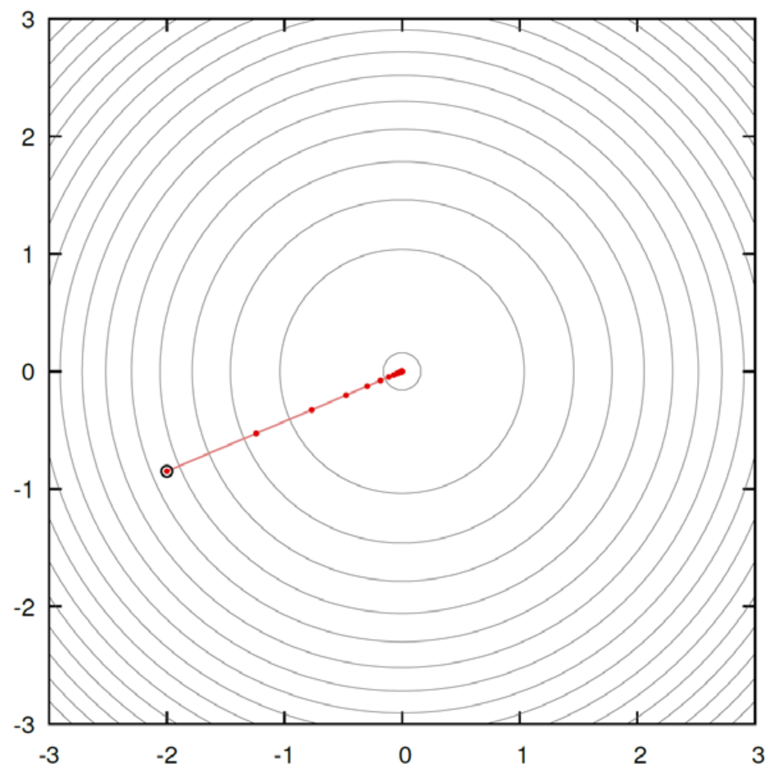
Harder !

Source: Dr. Francois Fleuret at EPFL

SGD Learning Rate: Spatial

- The gradient descent method makes a strong assumption about the magnitude of the "local curvature" to fix the step size, and about its isotropy so that the same step size makes sense in all directions.
- Nice (all features are equally important)

$\eta = 1.0e - 2$



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SGD Learning Rate: Spatial

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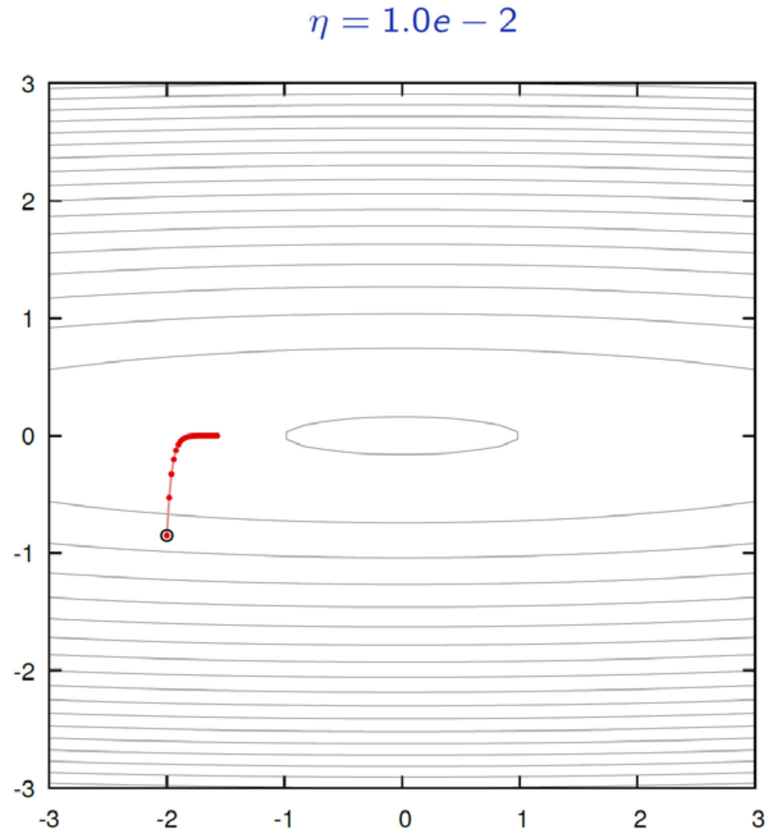

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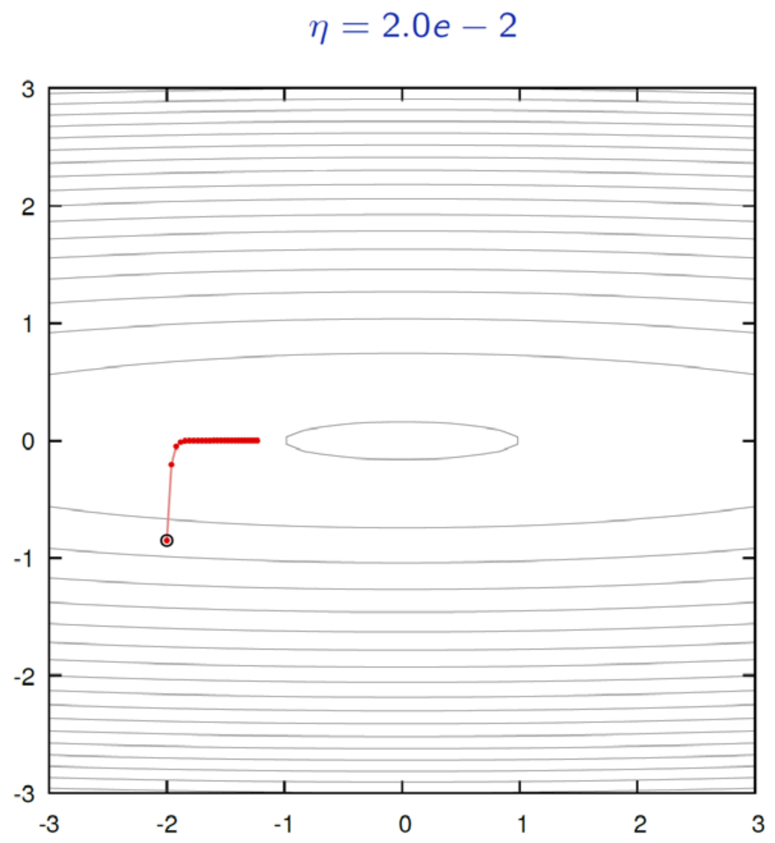

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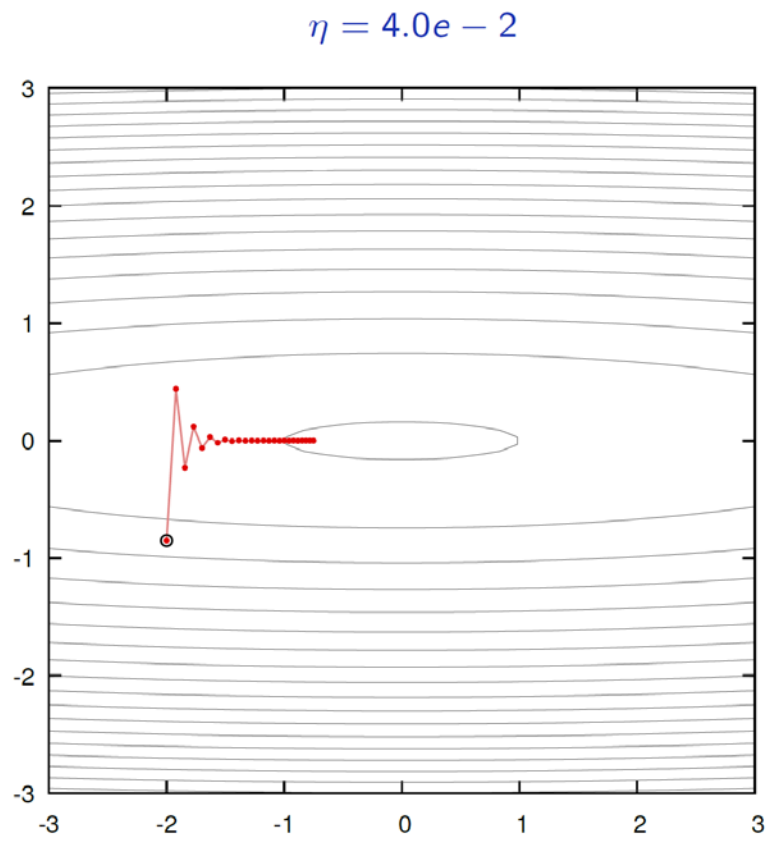

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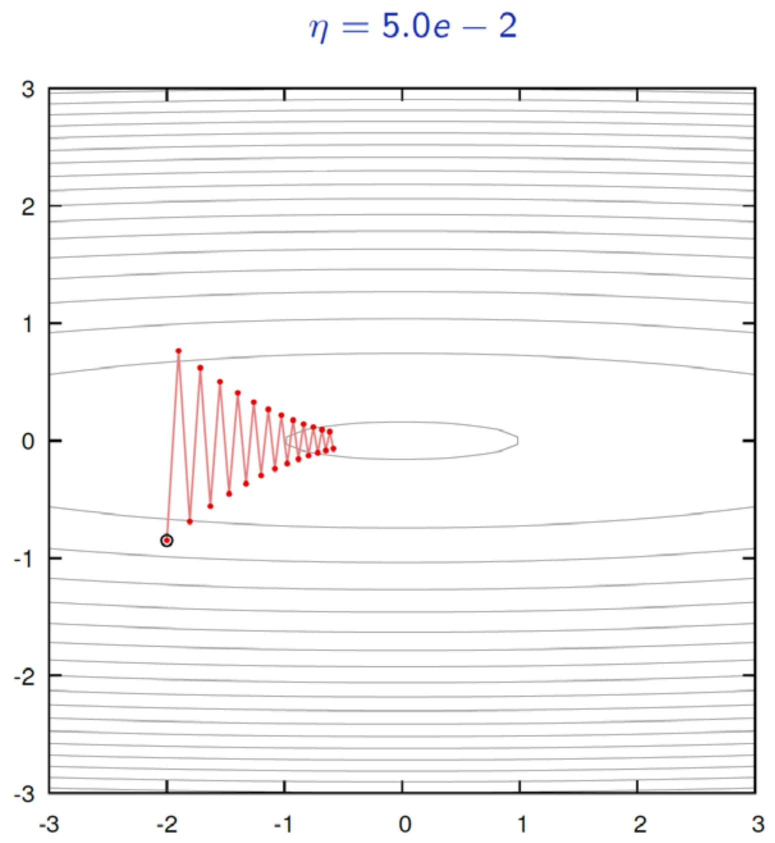

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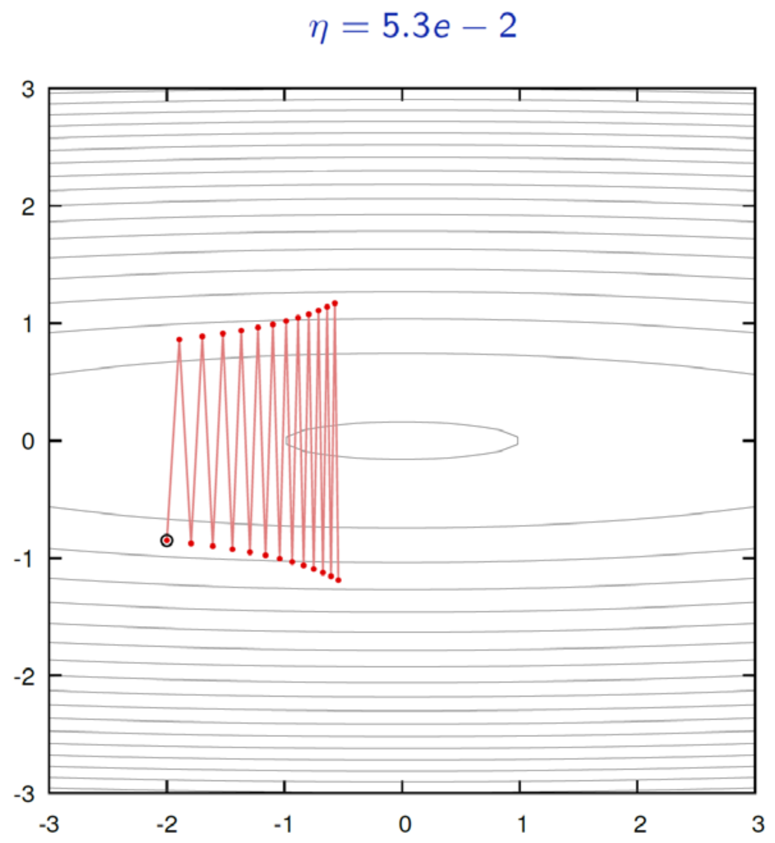


Source: Dr. Francois Fleuret at EPFL

SGD Learning Rate: Temporal

- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum
  - Gradually decay the learning rate to reduce the fluctuations

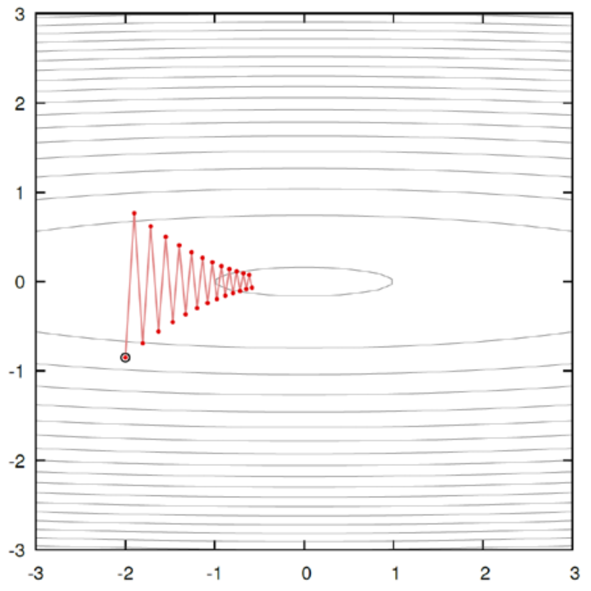
Adaptive Learning Rate Methods

- SDG

$$\theta_{t+1,i} = \theta_{t,i} - \eta \cdot g_{t,i}.$$

- Adagrad

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}.$$



  – $G_{t,ii}$ sum of the squares of the gradients
  – Perform smaller updates (i.e. low learning rates) for parameters ass occurring features, and
  – Perform larger updates (i.e. high learning rates) for parameters associated with infrequent features

- Deep-learning generally relies on a smarter use of the gradient, using statistics over its past values to make a “smarter step” with the current one.

Adaptive Learning Rate Methods

• Momentum	`tf.train.MomentumOptimizer`	Qian et al. "On the momentum term in gradient descent learning algorithms." 1999.
• Adagrad	`tf.train.AdagradOptimizer`	Duchi et al. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." 2011.
• Adadelta	`tf.train.AdadeltaOptimizer`	Zeiler et al. "ADADELTA: An Adaptive Learning Rate Method." 2012.
• Adam	`tf.train.AdamOptimizer`	Kingma et al. "Adam: A Method for Stochastic Optimization." 2014.
• RMSProp	`tf.train.RMSPropOptimizer`	

- Additional detail: http://ruder.io/optimizing-gradient-descent/

Source: 6.S191 Intro. to Deep Learning at MIT