CSC411: Optimization for Machine Learning

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Overview of Optimization

- An informal definition of optimization: Minimize (or maximize) some quantity.
- Applications:
  - Engineering: Minimize fuel consumption of an automobile
  - Economics: Maximize returns on an investment
  - Supply Chain Logistics: Minimize time taken to fulfill an order
  - Life: Maximize happiness
- More formally:
  - Goal: find $\theta^* =_\theta f(\theta)$ (possibly subject to constraints on θ)
  - $\theta \in \mathbb{R}^n$, optimization variable
  - $f : \mathbb{R}^n \to \mathbb{R}$, objective function

Optimization for Machine Learning

- Often in machine learning, we are interested in learning the parameters θ of a model.
- Goal: minimize some loss function
- For example, if we have some data (x, y), we may want to maximize $P(y|x, \theta)$.
- Equivalently, we can minimize $-\log P(y|x, \theta)$.
- We can also minimize other sorts of loss functions
- Log can help for numerical reasons

Gradient Descent: Motivation

- From calculus, we know that the minimum of f must lie at a point where $\frac{\partial f(\theta^*)}{\partial \theta} = 0$.
- Sometimes, we can solve this equation analytically for θ.
- Most of the time, we are not so lucky and must resort to iterative methods.

Brief review:

- Gradient: $\nabla_\theta f = (\frac{\partial f}{\partial \theta_1}, ..., \frac{\partial f}{\partial \theta_k})$.
- "Vector giving the direction (and rate) of steepest increase for f."

Outline of Gradient Descent Algorithm

Where η is the learning rate and T is the number of iterations:

- Initialize θ_0 randomly
- for $t = 1 : T$,
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

The learning rate shouldn't be too big (objective function will blow up) or too small (will take a long time to converge)

Gradient Descent with Momentum

We can introduce a momentum coefficient $\alpha \in [0, 1)$ so that the updates have "memory":

- Initialize θ_0 randomly
- Initialize δ_0 to the zero vector
- for $t = 1 : T$,
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f + \alpha \delta_{t-1}$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Momentum is a nice trick that can help speed up convergence. Generally we choose α between 0.8 and 0.95, but this is problem dependent.

Some convergence criteria

- Change in objective function value is close to zero: $|f(\theta_{t+1}) - f(\theta_t)| < \epsilon$
- Gradient norm is close to zero: $\|\nabla_\theta f\| < \epsilon$
- Validation error starts to increase (this is called *early stopping*)

Checkgrad

- When implementing the gradient computation for machine learning models, it's often difficult to know if our implementation of f and ∇f is correct.
- We can use finite-differences approximation to the gradient to help:

$$\frac{\partial f}{\partial \theta_i} \approx \frac{f((\theta_1, \ldots, \theta_i + \epsilon, \ldots, \theta_n)) - f((\theta_1, \ldots, \theta_i - \epsilon, \ldots, \theta_n))}{2\epsilon}$$

Why don't we always just use the finite differences approximation?

- slow: we need to recompute f twice for each parameter in our model.
- numerical issues

Stochastic Gradient Descent

- Any iteration of a gradient descent (or quasi-Newton) method requires that we sum over the entire dataset to compute the gradient.
- SGD idea: at each iteration, sub-sample a small amount of data (even just 1 point can work) and use that to estimate the gradient.
- Each update is noisy, but very fast!
- It can be shown that this method produces an unbiased estimator of the true gradient.
- This is the basis of optimizing ML algorithms with huge datasets (e.g., recent deep learning).

Stochastic Gradient Descent

- The reason SGD works is because similar data yields similar gradients, so if there is enough redundancy in the data, the noise from subsampling won't be so bad.
- SGD is very easy to implement compared to other methods, but the step sizes need to be tuned to different problems, whereas batch learning typically "just works".
- Tip 1: divide the log-likelihood estimate by the size of your mini-batches. This makes the learning rate invariant to mini-batch size.
- Tip 2: subsample without replacement so that you visit each point on each pass through the dataset (this is known as an epoch).

Definition of Convexity

A function f is convex if for any two points θ_1 and θ_2 and any $t \in [0, 1]$,

$$f(t\theta_1 + (1-t)\theta_2) \leq tf(\theta_1) + (1-t)f(\theta_2)$$

We can compose convex functions such that the resulting function is also convex:

- If f is convex, then so is αf for $\alpha \geq 0$
- If f_1 and f_2 are both convex, then so is $f_1 + f_2$

Why do we care about convexity?

- Any local minimum is a global minimum.
- This makes optimization a lot easier because we don't have to worry about getting stuck in a local minimum.

Examples of Convex Functions

- Quadratics
- Negative logarithms
- Cross-entropy objective function for logistic regression is also convex!

$$f(\theta) = -\sum_n y^{(n)} \log P(y = 1|x^{(n)}, \theta) + (1 - y^{(n)}) \log P(y = 0|x^{(n)}, \theta)$$

Examples of Convex Functions

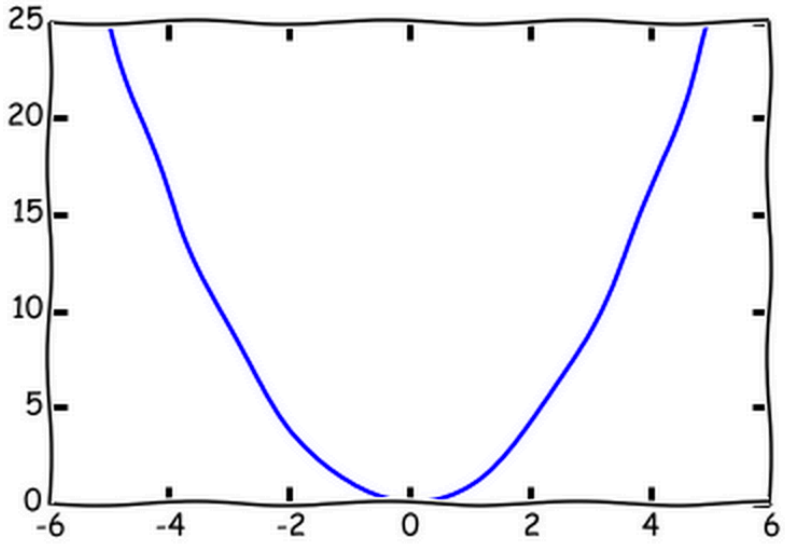
Quadratics

In [6]:

Slide Type -

```
import matplotlib.pyplot as plt
plt.xkcd()
theta = linspace(-5, 5)
f = theta**2
plt.plot(theta, f)
```

Out[6]: [<matplotlib.lines.Line2D at 0x3ceae90>]



Examples of Convex Functions

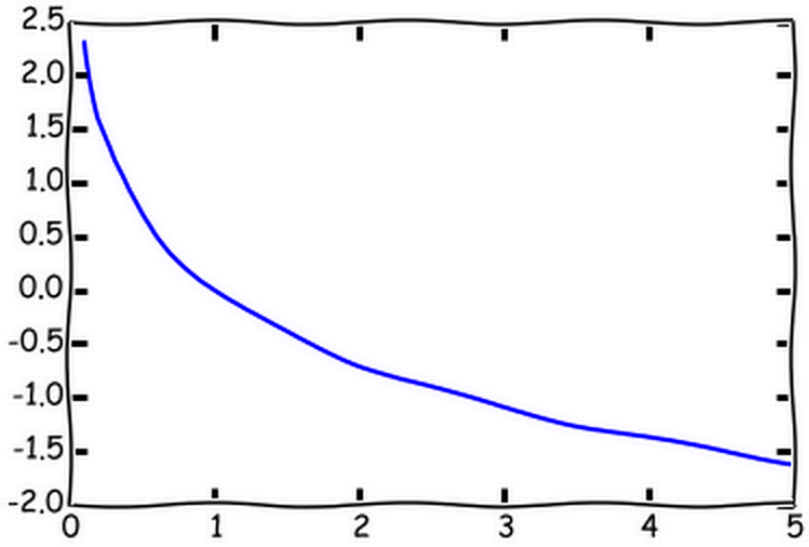
Negative logarithms

In [8]:

Slide Type -

```
import matplotlib.pyplot as plt
plt.xkcd()
theta = linspace(0.1, 5)
f = -np.log(theta)
plt.plot(theta, f)
```

Out[8]: [<matplotlib.lines.Line2D at 0x3ef4a10>]



Convexity for logistic regression

Cross-entropy objective function for logistic regression is also convex!

$f(\theta) = -\sum_n t^{(n)} \log p(y = 1|x^{(n)}, \theta) + (1 - t^{(n)}) \log p(y = 0|x^{(n)}, \theta)$

Plot of $-\log \sigma(\theta)$

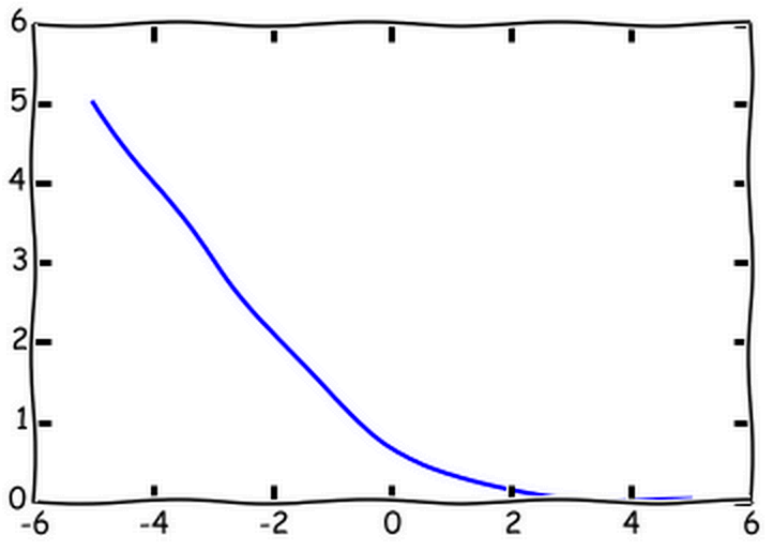
In [15]:

Slide Type -

```
def sigmoid(x):
    return 1 / (1 + np.exp(-x))

theta = linspace(-5, 5)
f = -np.log(sigmoid(theta))
plt.plot(theta, f)
```

Out[15]: [<matplotlib.lines.Line2D at 0x4c453d0>]



More on optimization

- *Automatic Differentiation* Modern technique (used in libraries like tensorflow, pytorch, etc) to efficiently compute the gradients required for optimization. A survey of these techniques can be found here: https://arxiv.org/pdf/1502.05767.pdf
- *Convex Optimization* by Boyd & Vandenberghe Book available for free online at http://www.stanford.edu/~boyd/cvxbook/
- *Numerical Optimization* by Nocedal & Wright Electronic version available from UofT Library

Cross-Validation

Cross-Validation: Why Validate?

So far:

Learning as Optimization

Goal: Optimize model complexity (for the task)
while minimizing under/overfitting

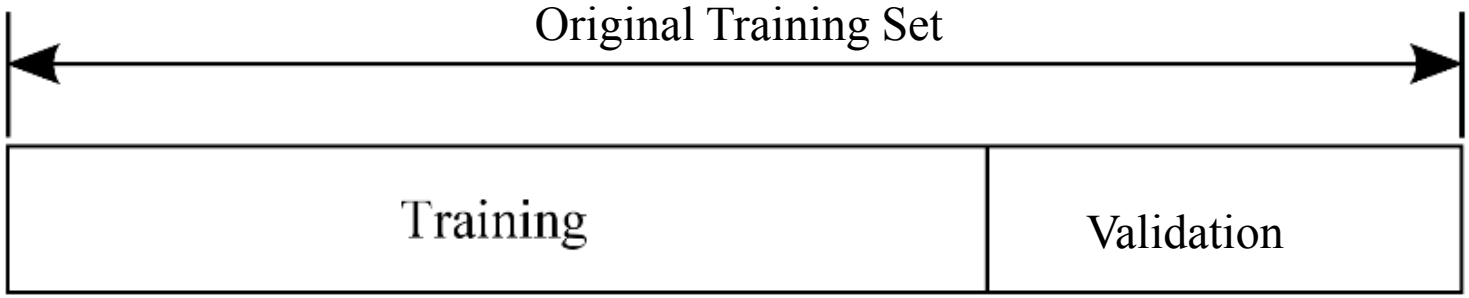
We want our model to **generalize well** without **overfitting**.

We can ensure this by **validating** the model.

Types of Validation

Hold-Out Validation: Split data into training and validation sets.

- Usually 30% as hold-out set.



Problems:

- Waste of dataset
- Estimation of error rate might be misleading

Types of Validation

- **Cross-Validation**: Random subsampling

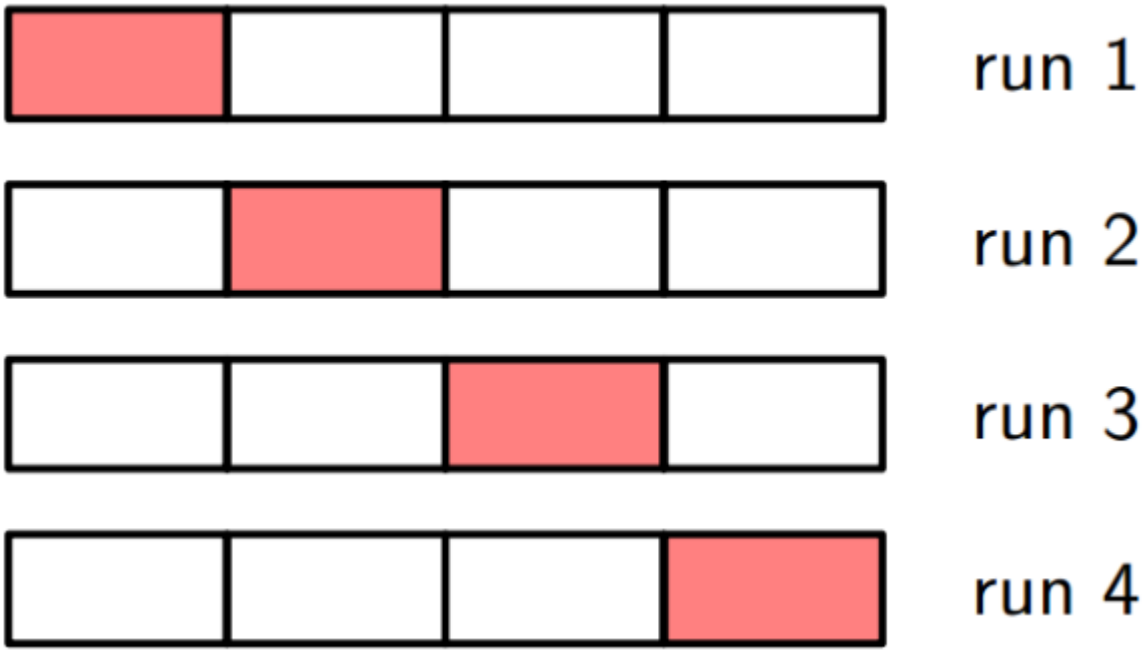


Figure from Bishop, C.M. (2006). *Pattern Recognition and Machine Learning*. Springer

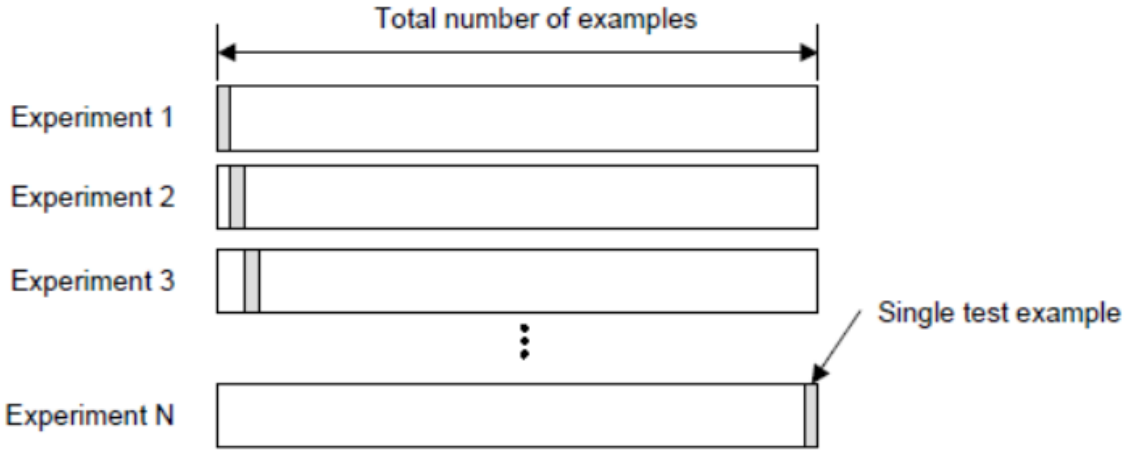
Problem:

- More **computationally expensive** than hold-out validation.

Variants of Cross-Validation

Leave-*p*-out: Use p examples as the validation set, and the rest as training; repeat for all configurations of examples.

e.g., for $p = 1$:

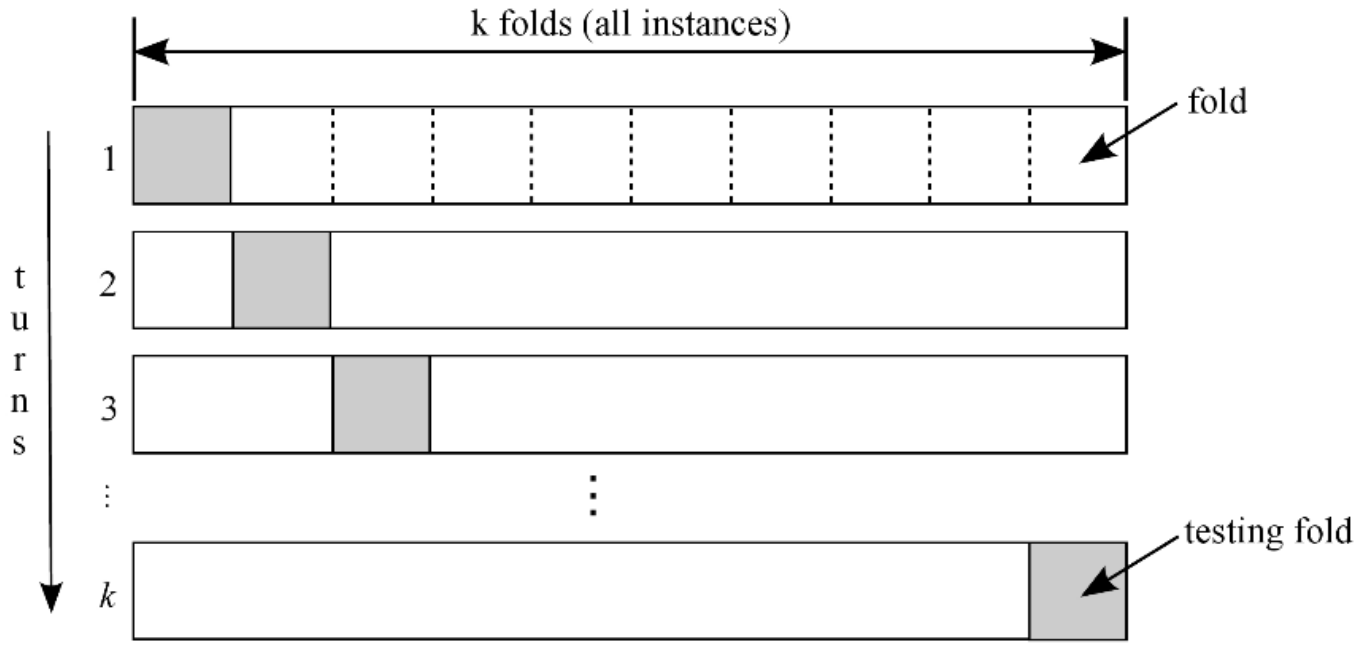


Problem:

- **Exhaustive**. We have to train and test $\binom{N}{p}$ times, where N is the # of training examples.

Variants of Cross-Validation

K-fold: Partition training data into K equally sized subsamples. For each fold, use the other K-1 subsamples as training data with the last subsample as validation.



K-fold Cross-Validation

- Think of it like leave-*p*-out but without combinatoric amounts of training/testing.

Advantages:

- All observations are used for both training and validation. Each observation is used for validation **exactly once**.
- **Non-exhaustive**: More tractable than leave-*p*-out

K-fold Cross-Validation

Problems:

- **Expensive** for large *N, K* (since we train/test *K* models on *N* examples).
  - But there are some efficient hacks to save time…
- Can still **overfit** if we validate too many models!
  - **Solution**: Hold out an additional test set before doing any model selection, and check that the best model performs well on this additional set (*nested cross-validation*). => Cross-Validception

Practical Tips for Using K-fold Cross-Val

Q: How many folds do we need?

A: With **larger** *K*, …

- Error estimation tends to be **more accurate**
- But, computation time will be **greater**

In practice:

- Usually use $\boldsymbol{K \approx 10}$
- BUT, larger dataset => choose **smaller *K***