**To get SGD off the ground, we don't just need software. Here are some basic statistical techniques that we pretty much always use...**

# Getting SGD Off The Ground II

## Basic Techniques We Always Use

CS6787 Lecture 3 — Spring 2024

# Overfitting, Generalization Error, and Regularization

# Minimizing Training Loss is Not our Real Goal

- Training loss looks like

$$h(w) = \frac{1}{N} \sum_{i=1}^{N} f(w; x_i)$$

- What we actually want to minimize is **expected loss on new examples**
  - Drawn from some real-world distribution $\phi$

$$\bar{h}(w) = \mathbf{E}_{x \sim \phi} \left[ f(w; x) \right]$$

  - Typically, assume the training examples were drawn from this distribution

# Overfitting

- Minimizing the training loss **doesn't generally minimize the expected loss** on new examples
  - They are two different objective functions after all
- Difference between the empirical loss on the training set and the expected loss on new examples is called the **generalization error**
- Even a model that has high accuracy on the training set can have terrible performance on new examples
  - Phenomenon is called **overfitting**

# Demo

# How to address overfitting

- **Many, many techniques** to deal with overfitting
  - Have varying computational costs
- But this is a systems course…so what can we do **with little or no extra computational cost?**
- Notice from the demo that **some loss functions do better than others**
  - Can we **modify our loss function** to prevent overfitting?

# Regularization

- Add an extra **regularization term** to the objective function

- Most popular type: **L2 regularization**

$$h(w) = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \sigma^2 \|w\|_2^2 = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \sigma^2 \sum_{k=1}^{d} x_k^2$$

- Also popular: **L1 regularization**

$$h(w) = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \gamma \|w\|_1 = \frac{1}{N}\sum_{i=1}^{N} f(w; x_i) + \gamma \sum_{k=1}^{d} \|x_k\|$$

# Benefits of Regularization

- **Cheap to compute**
  - For SGD and L2 regularization, there's just an extra scaling

$$w_{t+1} = (1 - 2\alpha_t\sigma^2)w_t - \alpha_t \nabla f(w_t; x_{i_t})$$

- **L2 regularization makes the objective strongly convex**
  - This makes it easier to get and prove bounds on convergence

- **Helps with overfitting**

# Demo

# How to choose the regularization parameter?

- One way is to use an independent **validation set** to estimate the test error, and set the regularization parameter manually so that it is high enough to avoid overfitting
  - This is what we saw in the demo

- But doing this naively can be **computationally expensive**
  - Need to re-run learning algorithm many times

- Yet another use case for **hyperparameter optimization**

# More general forms of regularization

- **Regularization** is used more generally to describe anything that helps prevent overfitting
  - By biasing learning by making some models more desirable *a priori*

- Many techniques that give throughput improvements also have a regularizing effect
  - Sometimes: a **win-win** of better statistical and hardware performance

# Early Stopping

# Asymptotically large training sets

- Setting 1: we have a distribution $\phi$ and we sample a very large (asymptotically infinite) number of points from it, then run stochastic gradient descent on that training set for only **N** iterations.

- Can our algorithm in this setting overfit?
  - **No, because its training set is asymptotically equal to the true distribution.**

- Can we compute this efficiently?
  - **No, because its training set is asymptotically infinitely large**

# Consider a second setting

- Setting 1: we have a distribution $\phi$ and we sample a very large (asymptotically infinite) number of points from it, then run stochastic gradient descent on that training set for only **N** iterations.

- Setting 2: we have a distribution $\phi$ and we sample **N** points from it, then run stochastic gradient descent using each of these points exactly once.

- What is the difference between the output of SGD in these two settings?
  - **Asymptotically, there's no difference!**
  - So SGD in Setting 2 will also never overfit

# Early Stopping

- Motivation: if we only use each training example once for SGD, then we can't overfit.

- So if we **only use each example a few times**, we probably won't overfit too much.

- **Early stopping**: just stop running SGD before it converges.

# Benefits of Early Stopping

- **Cheap to compute**
  - Literally just does less work
  - It seems like the technique was designed to make systems run faster
- **Helps with overfitting**
- **BE SURE TO TEST IT CORRECTLY!**

# Another class of technique: Acceleration and Momentum

# How does the step size affect convergence?

- Let's go back to gradient descent

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

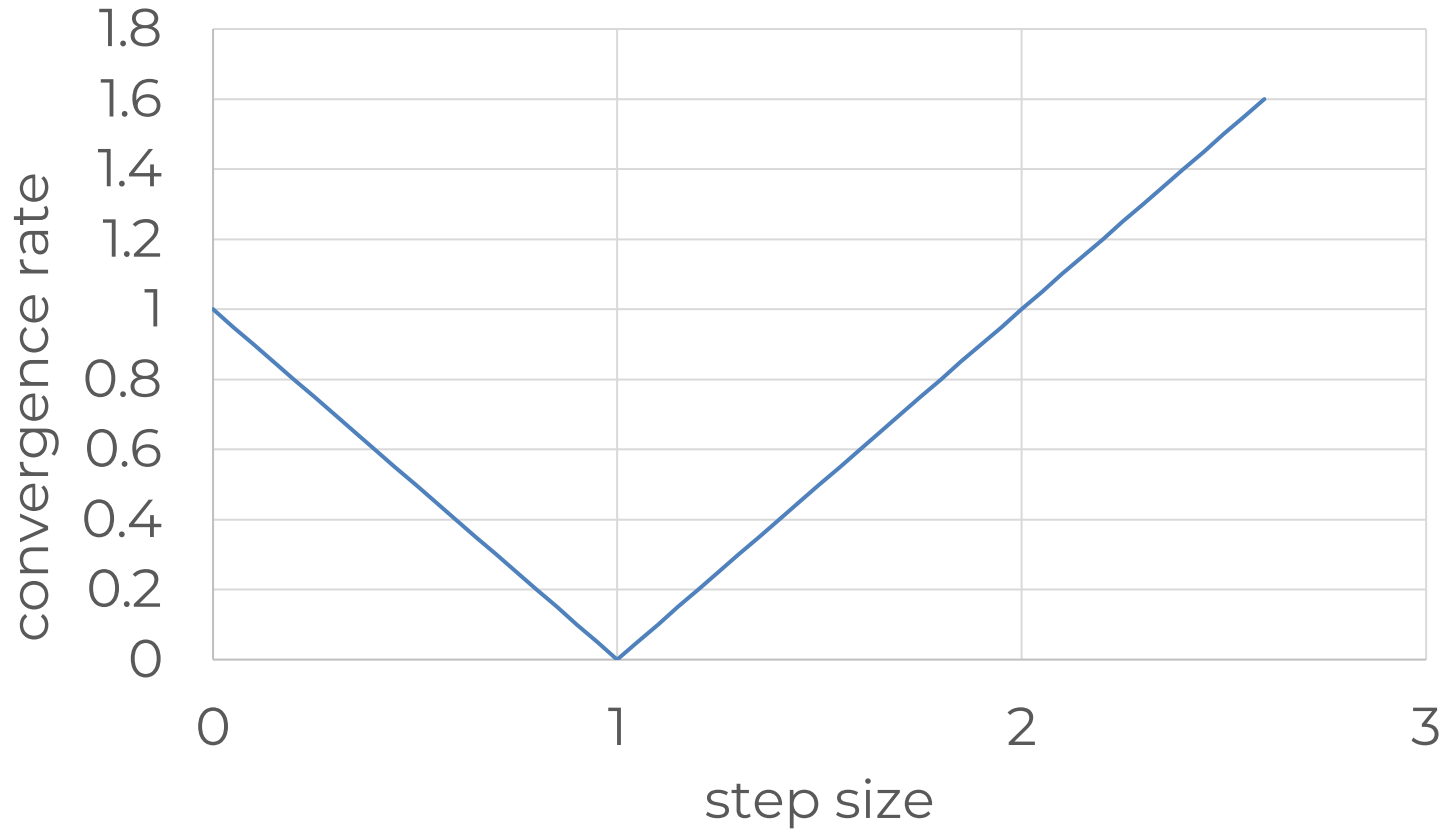
- Simplest possible case: a quadratic function

$$f(x) = \frac{1}{2}x^2$$

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

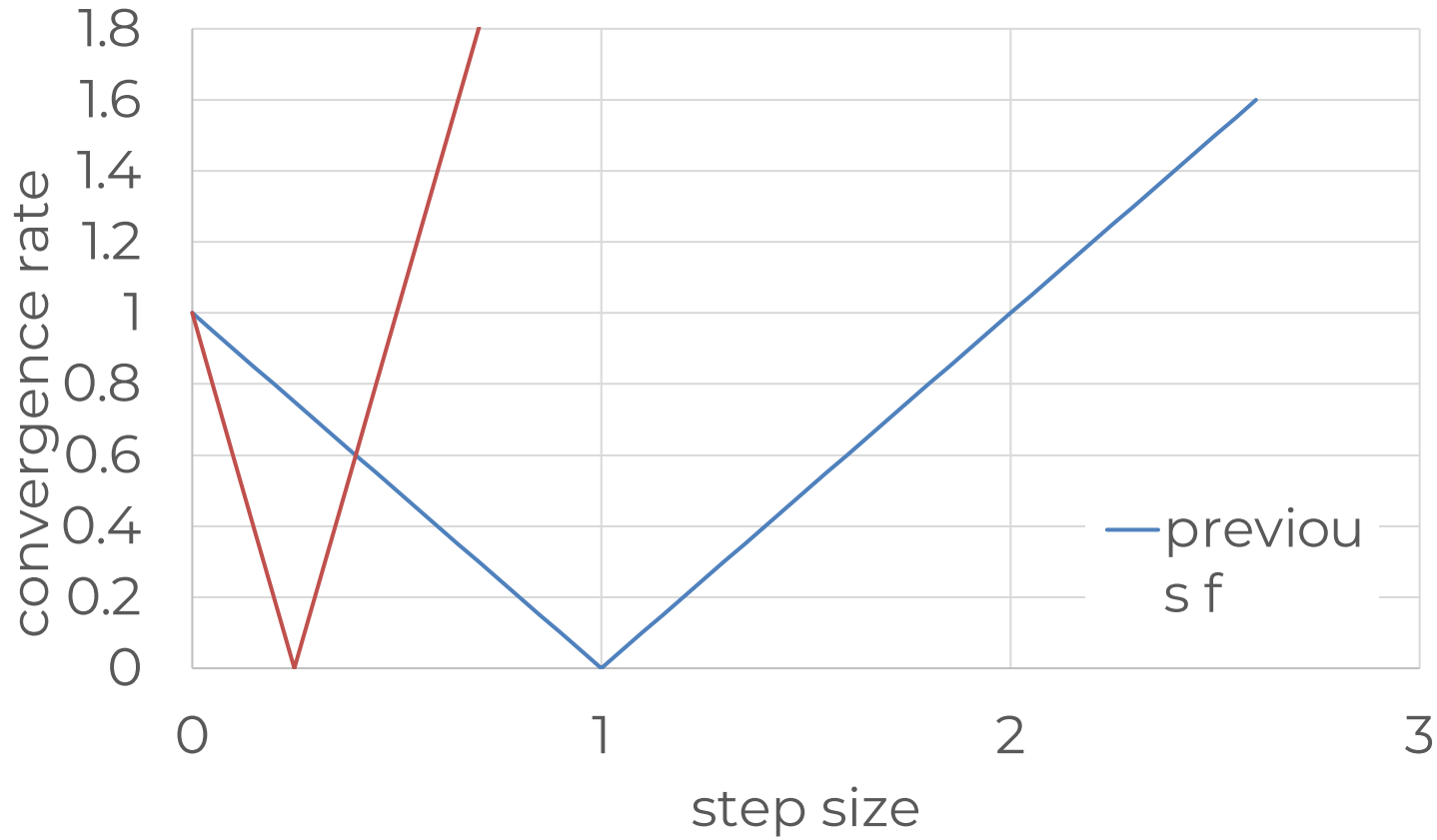
# Step size vs. convergence: graphically

$$|x_{t+1} - 0| = |1 - \alpha| \, |x_t - 0|$$



# What if the curvature is different?

$$f(x) = 2x^2 \qquad x_{t+1} = x_t - 4\alpha x_t = (1 - 4\alpha)x_t$$



# Step size vs. curvature

- For these one-dimensional quadratics, how we should set **the step size depends on the curvature**
  - More curvature → smaller ideal step size

- What about higher-dimensional problems?
  - Let's look at a really simple quadratic that's just a sum of our examples.

$$f(x, y) = \frac{1}{2}x^2 + 2y^2$$

# Simple two dimensional problem

$$f(x, y) = \frac{1}{2}x^2 + 2y^2$$

- Gradient descent:

$$\begin{bmatrix} x_{t+1} \\ y_{t+1} \end{bmatrix} = \begin{bmatrix} x_t \\ y_t \end{bmatrix} - \alpha \begin{bmatrix} x_t \\ 4y_t \end{bmatrix}$$

$$= \begin{bmatrix} 1-\alpha & 0 \\ 0 & 1-4\alpha \end{bmatrix} \begin{bmatrix} x_t \\ y_t \end{bmatrix}$$

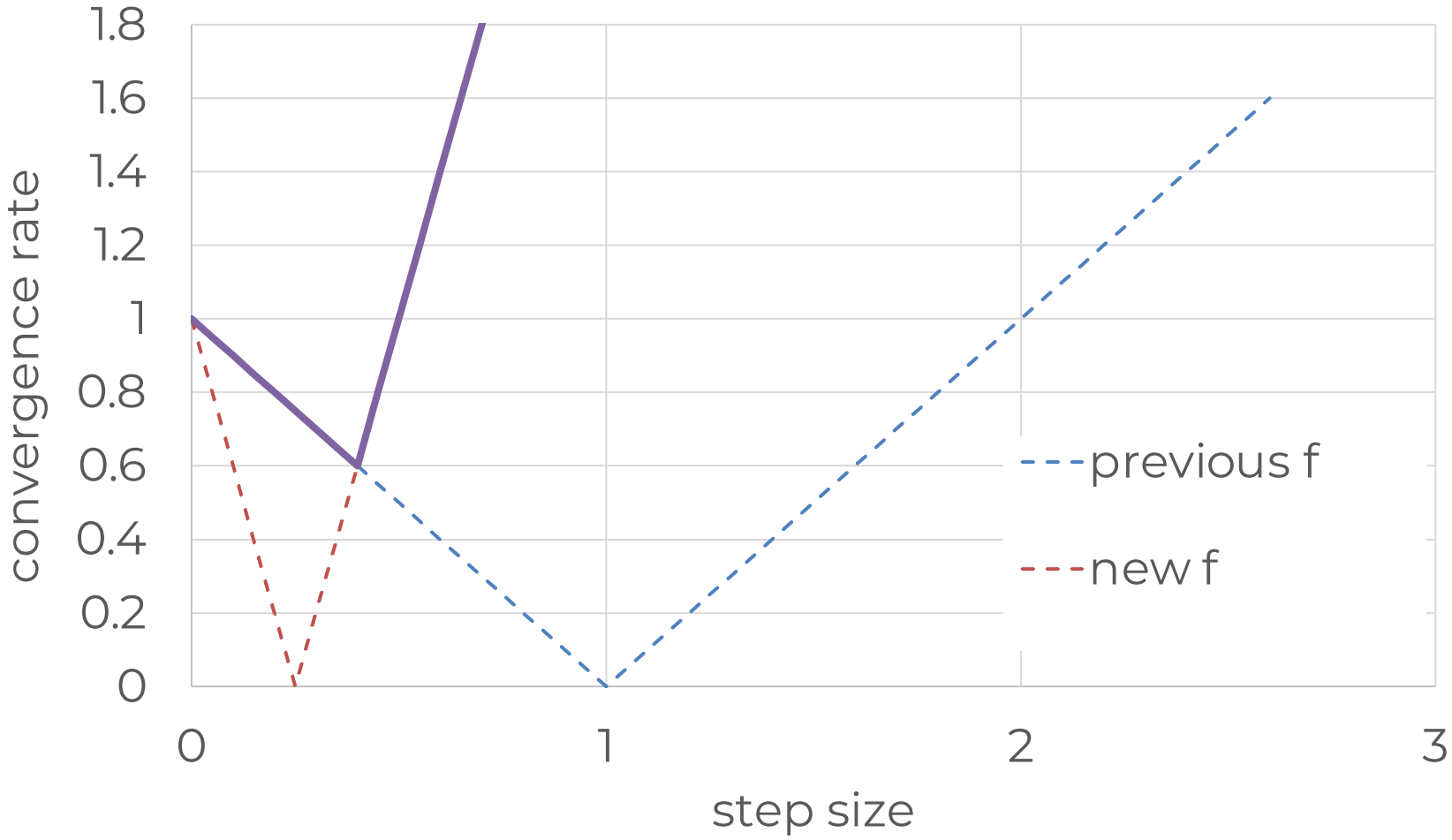
# What's the convergence rate?

- Look at the worst-case contraction factor of the update

$$\max_{x,y} \frac{\left\| \begin{bmatrix} 1-\alpha & 0 \\ 0 & 1-4\alpha \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right\|}{\left\| \begin{bmatrix} x \\ y \end{bmatrix} \right\|} = \max(|1-\alpha|, |1-4\alpha|)$$

- Contraction is maximum of previous two values.

# Convergence of two-dimensional quadratic



# What does this example show?

- We'd like to set the step size larger for dimension with less curvature, and smaller for the dimension with more curvature.

- But we can't, because there is **only a single step-size parameter**.

- There's a **trade-off**
  - Optimal convergence rate is **substantially worse than** what we'd get in each scenario individually — individually we converge in one iteration.

# For general quadratics

- For PSD symmetric A,

$$f(x) = \frac{1}{2} x^T A x$$

- Gradient descent has update step

$$x_{t+1} = x_t - \alpha A x_t = (I - \alpha A) x_t$$

- What does the convergence rate look like in general?

# Convergence rate for general quadratics

$$\begin{aligned}
\max_x \frac{\|(I-\alpha A)x\|}{\|x\|} &= \max_x \frac{1}{\|x\|} \left\| \left( I - \alpha \sum_{i=1}^{n} \lambda_i u_i u_i^T \right) x \right\| \\
&= \max_x \frac{\left\| \sum_{i=1}^{n} (1-\alpha\lambda_i) u_i u_i^T x \right\|}{\left\| \sum_{i=1}^{n} u_i u_i^T x \right\|} \\
&= \max_i |1-\alpha\lambda_i| \\
&= \max(1-\alpha\lambda_{\min}, \alpha\lambda_{\max}-1)
\end{aligned}$$

# Optimal convergence rate

- Minimize:

$$\max(1 - \alpha\lambda_{\min}, \alpha\lambda_{\max} - 1)$$

- Optimal value occurs when

$$1 - \alpha\lambda_{\min} = \alpha\lambda_{\max} - 1 \Rightarrow \alpha = \frac{2}{\lambda_{\max} + \lambda_{\min}}$$

- Optimal rate is

$$\max(1 - \alpha\lambda_{\min}, \alpha\lambda_{\max} - 1) = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$

# What affects this optimal rate?

$$\begin{aligned}\text{rate} &= \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \\ &= \frac{\lambda_{\max}/\lambda_{\min} - 1}{\lambda_{\max}/\lambda_{\min} + 1} \\ &= \frac{\kappa - 1}{\kappa + 1}.\end{aligned}$$

- Here, $\kappa$ is called the **condition number** of the matrix **A**.

$$\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$$

- Problems with larger condition numbers converge slower.
  - Called **poorly conditioned**.

# Poorly conditioned problems

- Intuitively, these are problems that are **highly curved in some directions but flat in others**

- Happens pretty often in machine learning
  - Measure something unrelated → low curvature in that direction
  - Also affects stochastic gradient descent

- **How do we deal with this?**

# Momentum

# Motivation

- Can we tell the difference between the curved and flat directions using information that is already available to the algorithm?

- Idea: in the one-dimensional case, if the gradients are **reversing sign**, then the step size is too large
  - Because we're **over-shooting the optimum**
  - And if the gradients stay in the same direction, then step size is too small

- Can we leverage this to make steps smaller when gradients reverse sign and larger when gradients are consistently in the same direction?

# Polyak Momentum

- Add extra **momentum term** to gradient descent

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

- Intuition: if current gradient step is in same direction as previous step, then move a little further in that direction.
  - And if it's in the opposite direction, move less far.

- Also known as the **heavy ball method**.

# Momentum for 1D Quadratics

$$f(x) = \frac{\lambda}{2}x^2$$

- Momentum gradient descent gives

$$\begin{aligned} x_{t+1} &= x_t - \alpha\lambda x_t + \beta(x_t - x_{t-1}) \\ &= (1 + \beta - \alpha\lambda)x_t - \beta x_{t-1} \end{aligned}$$

# Characterizing momentum for 1D quadratics

- Start with $x_{t+1} = (1 + \beta - \alpha\lambda)x_t - \beta x_{t-1}$

- Trick: let $x_t = \beta^{t/2} z_t$

$$\beta^{(t+1)/2} z_{t+1} = (1 + \beta - \alpha\lambda)\beta^{t/2} z_t - \beta \cdot \beta^{(t-1)/2} z_{t-1}$$

$$z_{t+1} = \frac{1 + \beta - \alpha\lambda}{\sqrt{\beta}} z_t - z_{t-1}$$

# Characterizing momentum (continued)

- Let

$$u = \frac{1 + \beta - \alpha\lambda}{2\sqrt{\beta}}$$

- Then we get the simplified characterization

$$z_{t+1} = 2uz_t - z_{t-1}$$

- This is a degree-***t*** polynomial in **u**

# Chebyshev Polynomials

- If we initialize such that $z_0 = 1, z_1 = u$ then these are a special family of polynomials called the **Chebyshev polynomials**

$$z_{t+1} = 2uz_t - z_{t-1}$$

- Standard notation:

$$T_{t+1}(u) = 2uT_t(u) - T_{t-1}(u)$$

- These polynomials have an important property: for all **t**

$$-1 \leq u \leq 1 \Rightarrow -1 \leq z_t \leq 1$$

# To see why they are bounded...

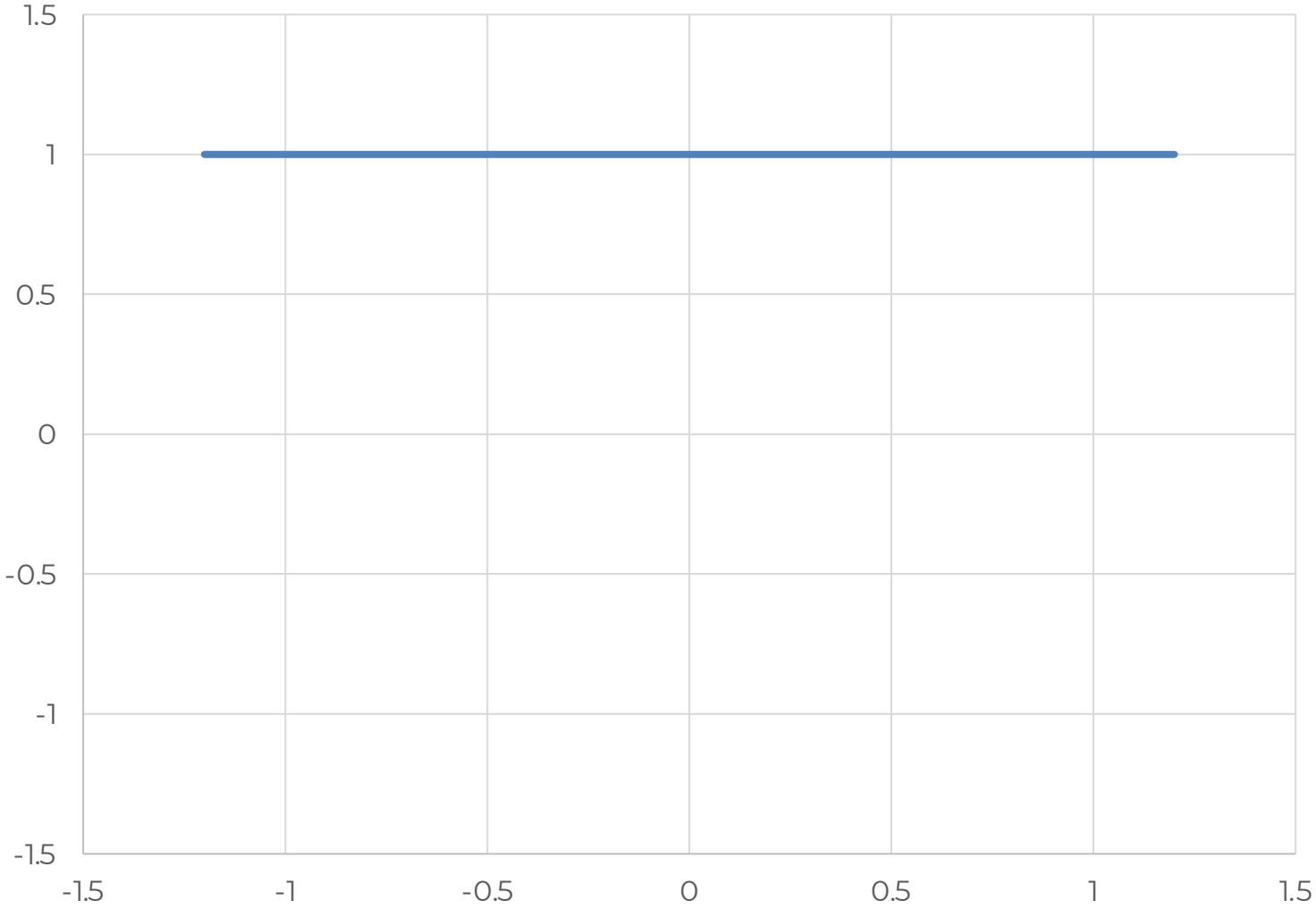
- **Chebyshev polynomials** $z_0 = 1,\ z_1 = u$

$$z_{t+1} = 2uz_t - z_{t-1}$$

- We can write them in terms of trig functions

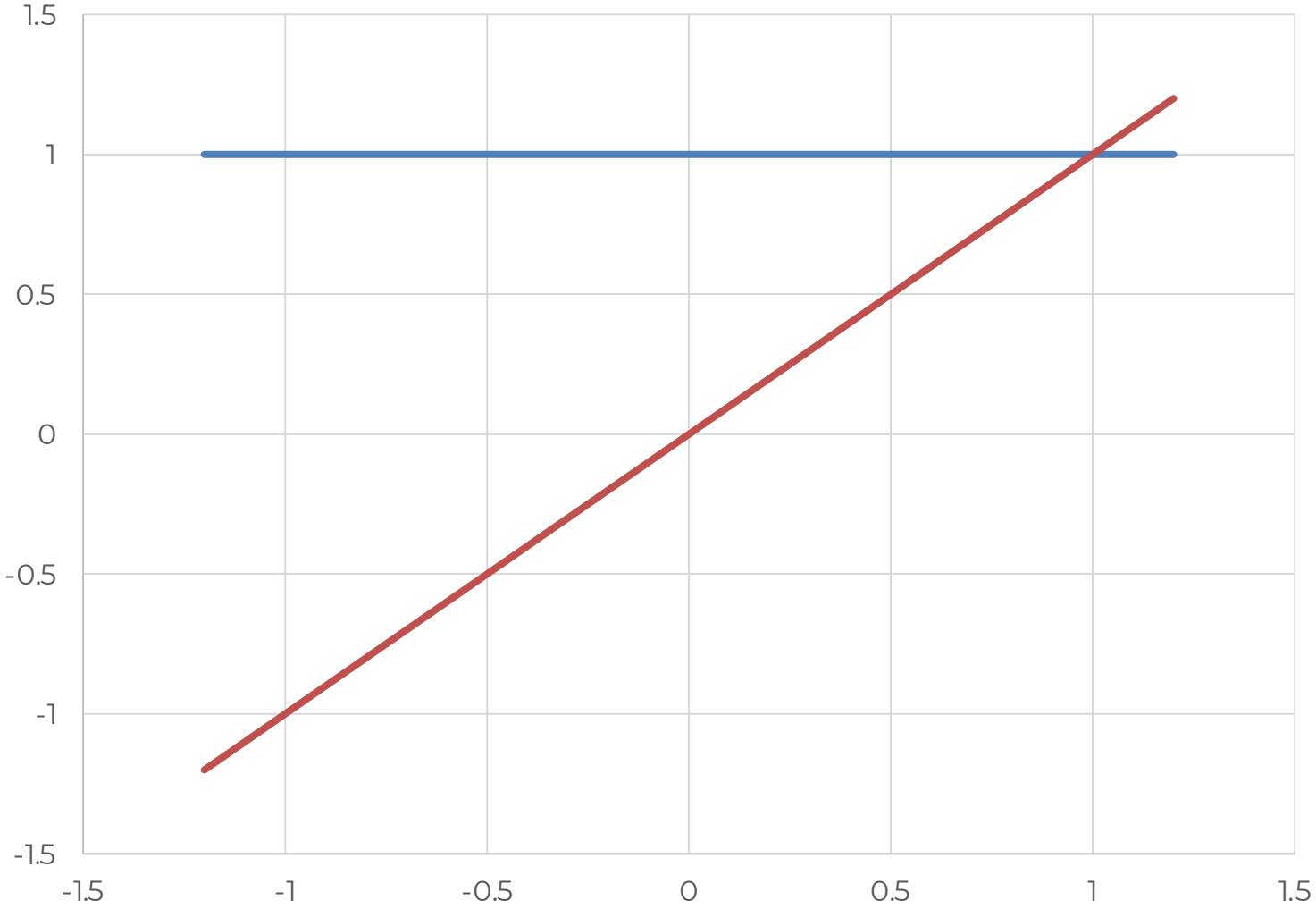
$$\cos((t+1)\theta) = \cos(\theta)\cos(t\theta) - \sin(\theta)\sin(t\theta)$$
$$\cos((t-1)\theta) = \cos(\theta)\cos(t\theta) + \sin(\theta)\sin(t\theta),$$
$$\underbrace{\cos((t+1)\theta)}_{T_{t+1}(u)} = 2\underbrace{\cos(\theta)}_{u}\underbrace{\cos(t\theta)}_{T_t(u)} - \underbrace{\cos((t-1)\theta)}_{T_{t-1}(u)}.$$

# Chebyshev Polynomials



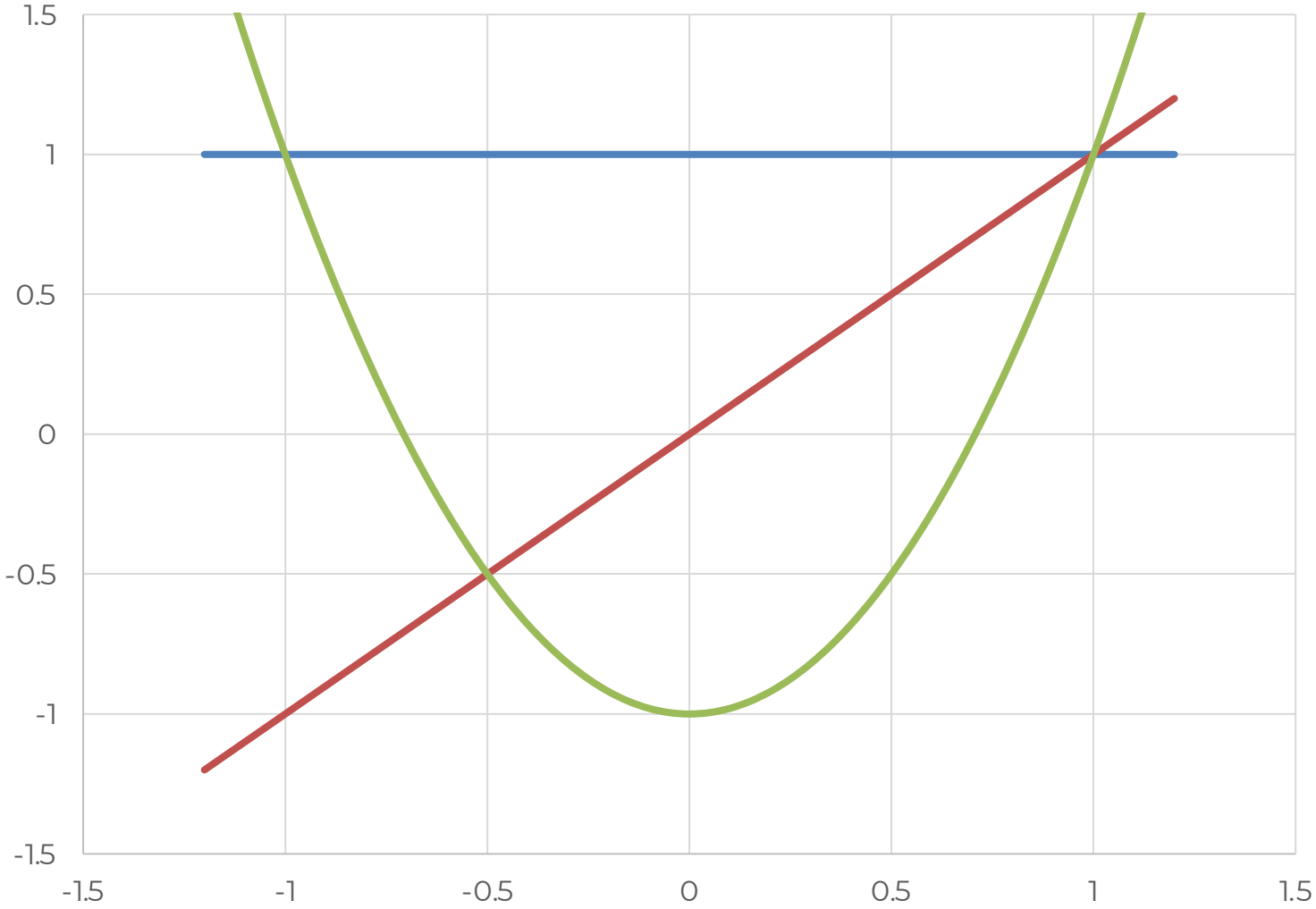

$$T_0(u) = 1$$

# Chebyshev Polynomials



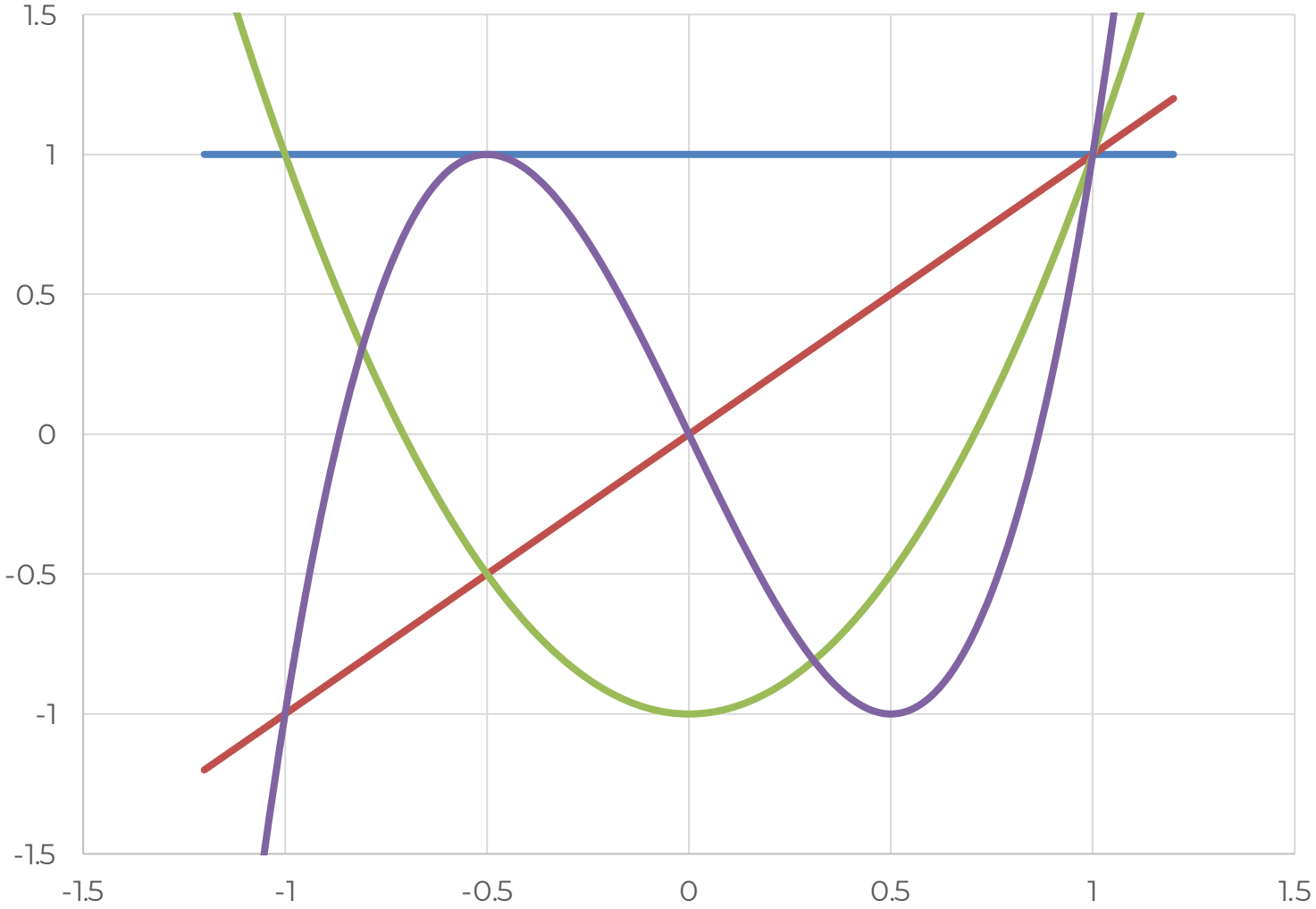

$$T_1(u) = u$$

# Chebyshev Polynomials

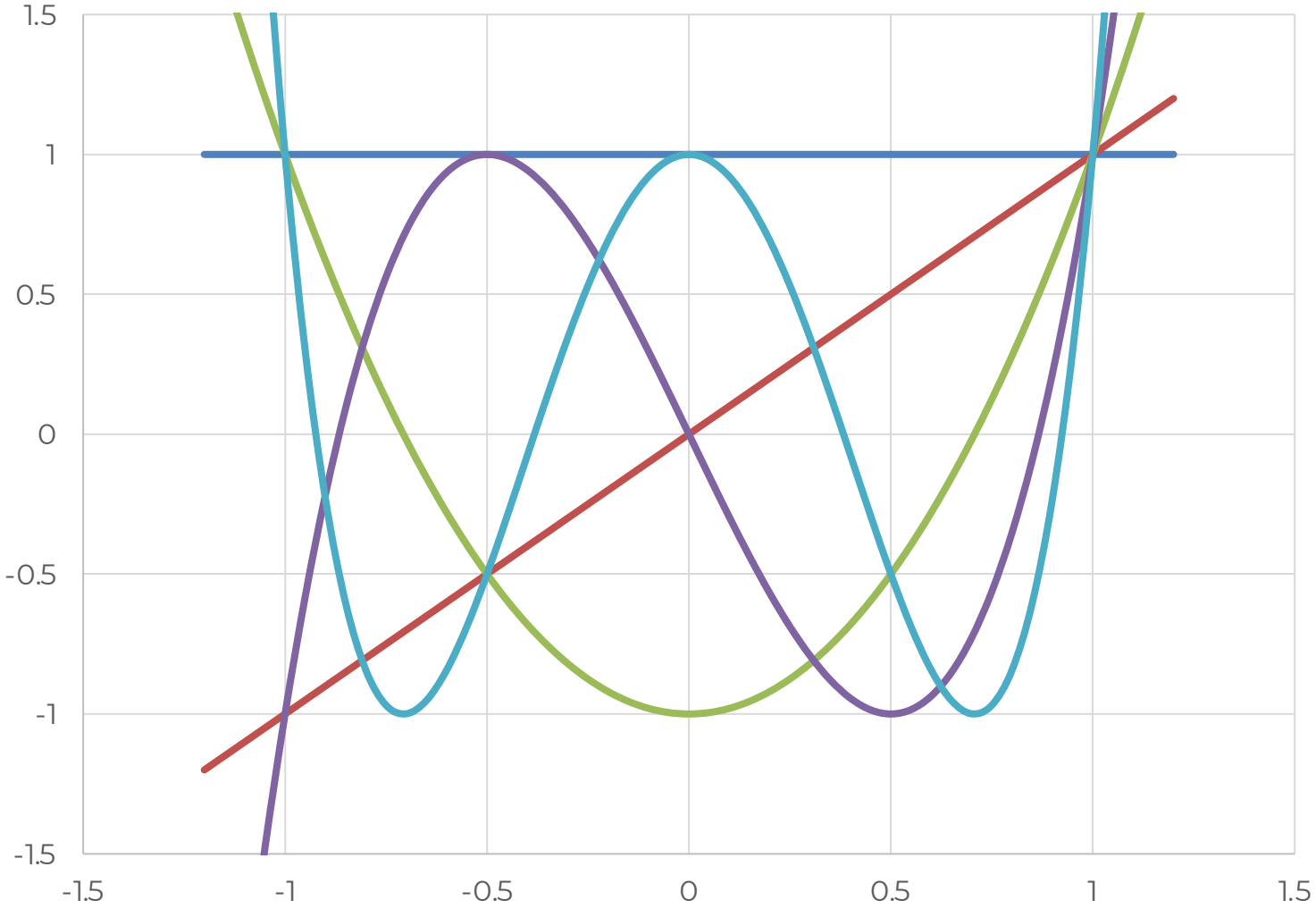



$$T_2(u) = 2u^2 - 1$$

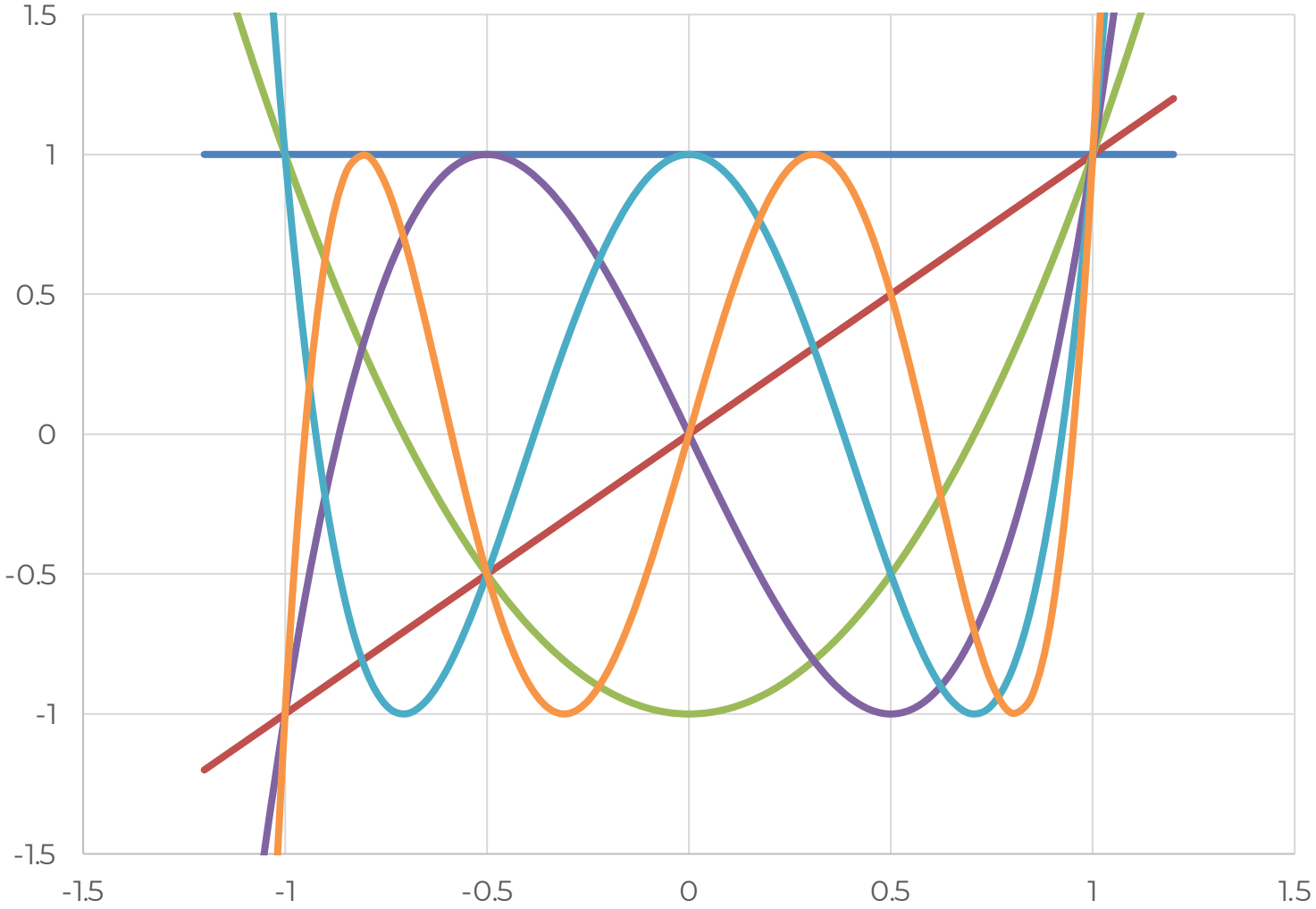
# Chebyshev Polynomials



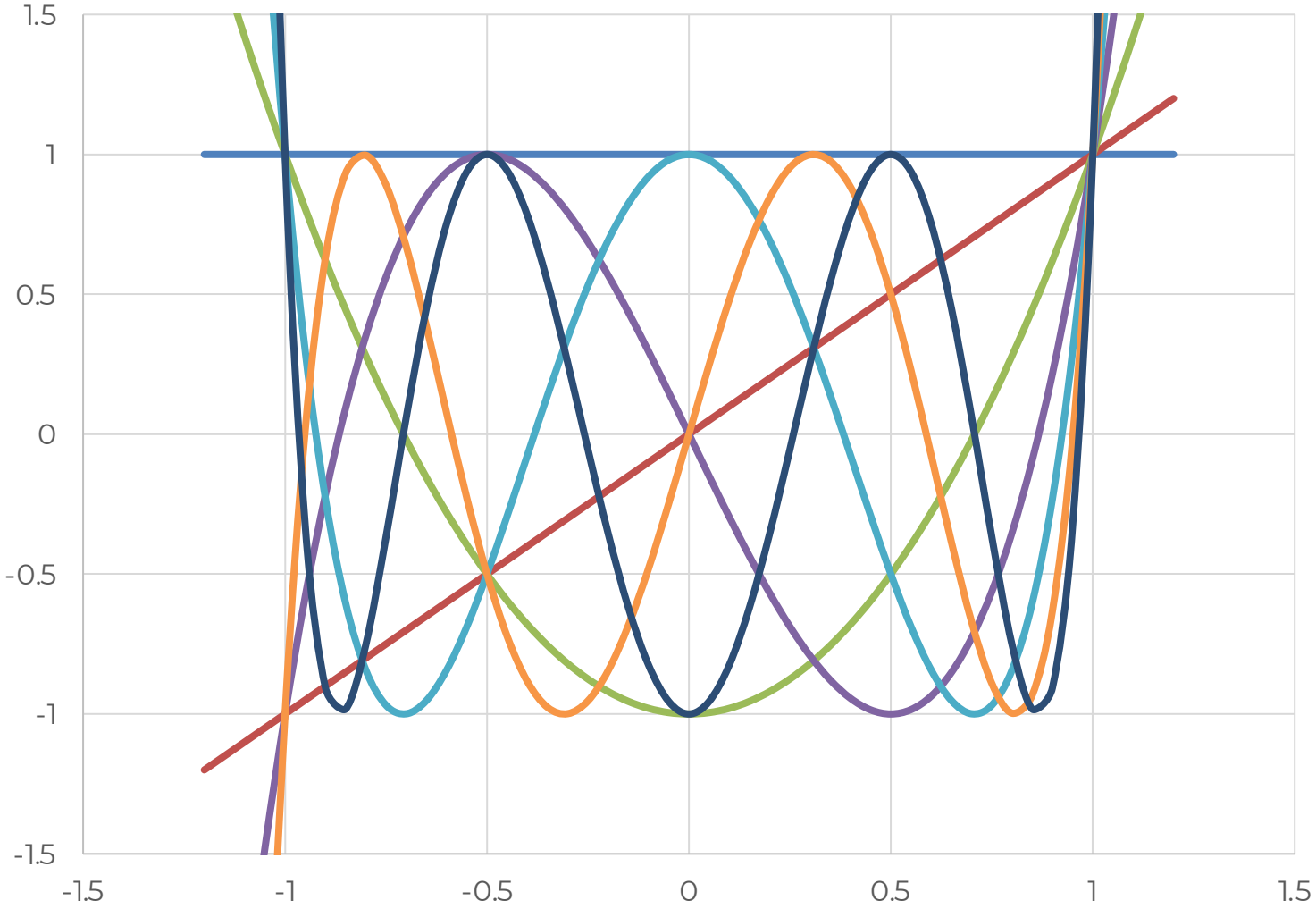
# Chebyshev Polynomials



# Chebyshev Polynomials



# Chebyshev Polynomials



# Characterizing momentum (continued)

- What does this mean for our 1D quadratics?
  - Recall that we let $x_t = \beta^{t/2} z_t$

$$x_t = \beta^{t/2} \cdot x_0 \cdot T_t(u)$$
$$= \beta^{t/2} \cdot x_0 \cdot T_t\left(\frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}}\right)$$

- So

$$-1 \leq \frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}} \leq 1 \Rightarrow |x_t| \leq \beta^{t/2} |x_0|$$

# Consequences of momentum analysis

- Convergence rate depends **only on momentum parameter β**
  - Not on step size or curvature.

- We **don't need to be that precise in setting the step size**
  - It just needs to be within a window
  - Pointed out in "*YellowFin and the Art of Momentum Tuning*" by Zhang et. al.

- If we have a multidimensional quadratic problem, the **convergence rate will be the same in all directions**
  - This is different from the gradient descent case where we had a trade-off

# Choosing the parameters

- How should we **set the step size and momentum parameter** if we only have bounds on $\lambda$ ?

- Need:
$$-1 \leq \frac{1+\beta-\alpha\lambda}{2\sqrt{\beta}} \leq 1$$

- Suffices to have:

$$-1 = \frac{1+\beta-\alpha\lambda_{\max}}{2\sqrt{\beta}} \text{ and } \frac{1+\beta-\alpha\lambda_{\min}}{2\sqrt{\beta}} = 1$$

# Choosing the parameters (continued)

- Adding both equations:

$$0 = \frac{2 + 2\beta - \alpha\lambda_{\max} - \alpha\lambda_{\min}}{2\sqrt{\beta}}$$

$$0 = 2 + 2\beta - \alpha\lambda_{\max} - \alpha\lambda_{\min}$$

$$\alpha = \frac{2 + 2\beta}{\lambda_{\max} + \lambda_{\min}}$$

# Choosing the parameters (continued)

- Subtracting both equations:

$$\frac{1+\beta-\alpha\lambda_{\min}-1-\beta+\alpha\lambda_{\max}}{2\sqrt{\beta}}=2$$

$$\frac{\alpha(\lambda_{\max}-\lambda_{\min})}{2\sqrt{\beta}}=2$$

# Choosing the parameters (continued)

- Combining these results: $\alpha = \dfrac{2+2\beta}{\lambda_{\max}+\lambda_{\min}}$ $\dfrac{\alpha(\lambda_{\max}-\lambda_{\min})}{2\sqrt{\beta}} = 2$

$$\frac{2+2\beta}{\lambda_{\max}+\lambda_{\min}} \cdot \frac{(\lambda_{\max}-\lambda_{\min})}{2\sqrt{\beta}} = 2$$

$$0 = 1 - 2\sqrt{\beta}\frac{\lambda_{\max}+\lambda_{\min}}{\lambda_{\max}-\lambda_{\min}} + \beta$$

# Choosing the parameters (continued)

- Quadratic formula: $0 = 1 - 2\sqrt{\beta}\frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} + \beta$

$$\sqrt{\beta} = \frac{\kappa+1}{\kappa-1} - \sqrt{\left(\frac{\kappa+1}{\kappa-1}\right)^2 - 1}$$

$$= \frac{\kappa+1}{\kappa-1} - \sqrt{\frac{4\kappa}{\kappa^2 - 2\kappa + 1}}$$

$$= \frac{\kappa+1}{\kappa-1} - \frac{2\sqrt{\kappa}}{\kappa-1} = \frac{\left(\sqrt{\kappa}-1\right)^2}{\kappa-1} = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$$

# Gradient Descent versus Momentum

- Recall: gradient descent had a convergence rate of

$$\frac{\kappa - 1}{\kappa + 1}$$

- But with momentum, the optimal rate is

$$\sqrt{\beta} = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

- This is called **convergence at an accelerated rate**

# Demo

# Setting the parameters

- How do we set the momentum in practice for machine learning?

- One method: **hyperparameter optimization**

- Another method: just set $\beta = 0.9$
  - Works across a range of problems
  - Actually quite popular in deep learning

# Nesterov momentum

# What about more general functions?

- Previous analysis was for quadratics
- Does this work for general convex functions?
- Answer: **not in general**
  - We need to do something slightly different

# Nesterov Momentum

- Slightly different rule

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

- Main difference: separate the momentum state from the point that we are calculating the gradient at.

# Nesterov Momentum Analysis

- Converges at an accelerated rate **for ANY convex problem**

$$\sqrt{\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}}}$$

- Optimal assignment of the parameters:

$$\alpha = \frac{1}{\lambda_{\max}}, \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$$

# Nesterov Momentum is Also Very Popular

- People use it in practice for deep learning all the time
- Significant speedups in practice

# Demo

# What about network architectures?

- All our above analysis was for **gradient descent**
  - Looking at how we minimize the objective

- But the structure of the hypothesis class (the network architecture) is just as important for optimization
  - We'll see two examples of network arch on **Wednesday**

- Also note that **Programming Assignment 1 is out.**