Optimization fundamentals

L101: Machine Learning for Language Processing

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Previous lecture

Logistic regression parameter learning:

$$w^\star = \arg\min_w \sum_{(x,y)\in D} -y \log \sigma(w \cdot \phi(x)) - (1-y)\log(1-\sigma(w\cdot\phi(x)))$$

Supervised machine learning algorithms typically involve optimizing a loss over the training data:

$$w^\star = \arg\min_w L(w;\mathcal{D}), w \in \Re^k$$

This is an instance of **numerical optimization**, i.e. optimize the value of a function with respect to some parameters.

A scientific field of its own; this lecture just gives some useful pointers

Types of optimization problems

Continuous: $$x^\star = \arg\min_x f(x), x \in \Re^k$$

Discrete: $$x^\star = \arg\min_x L(x), x \in \mathbb{Z}^k$$

Sounds rare in NLP?

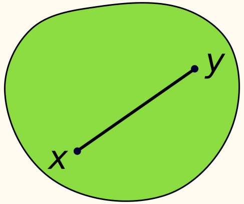
Inference in classification/structured prediction: a label is either applied or not

Constraints: $$x^\star = \arg\min_x L(x), c(x) \geq 0$$

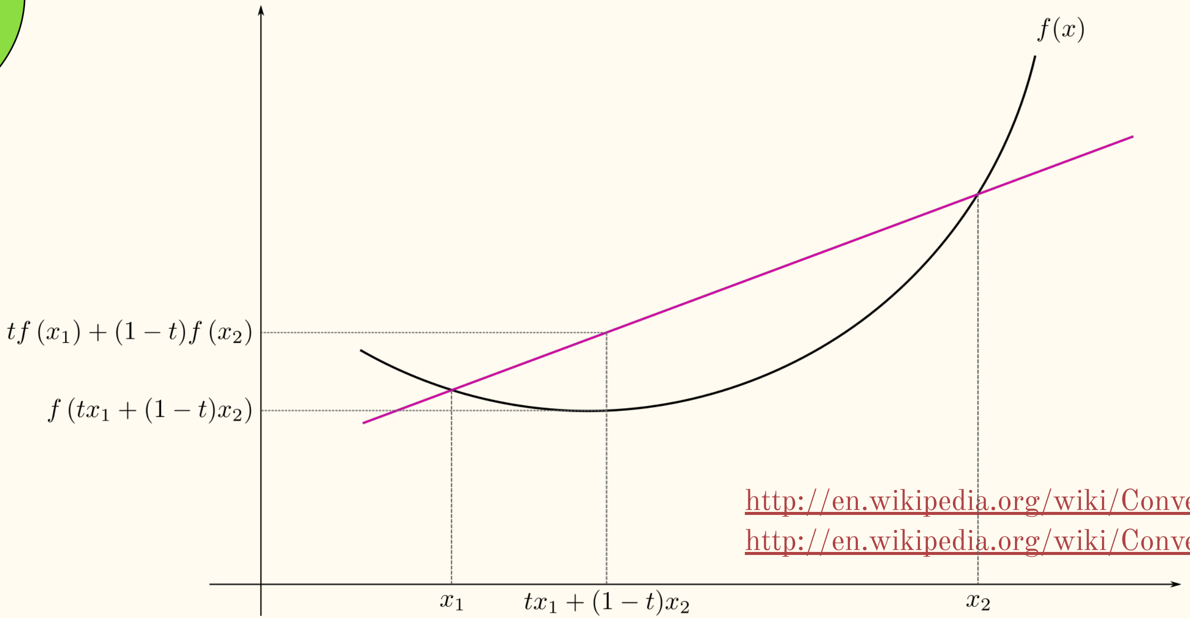
Examples: SVM parameter training, enforcing constraints on the output graph

Convexity

For sets:



$$\forall x, y \in S : ax + (1-a)y \in S, a \in [0,1]$$



For functions:

If *f* concave, -*f* is convex

For sets the relation is more complicated

http://en.wikipedia.org/wiki/Convex_set, http://en.wikipedia.org/wiki/Convex_function

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2), t \in [0,1]$$

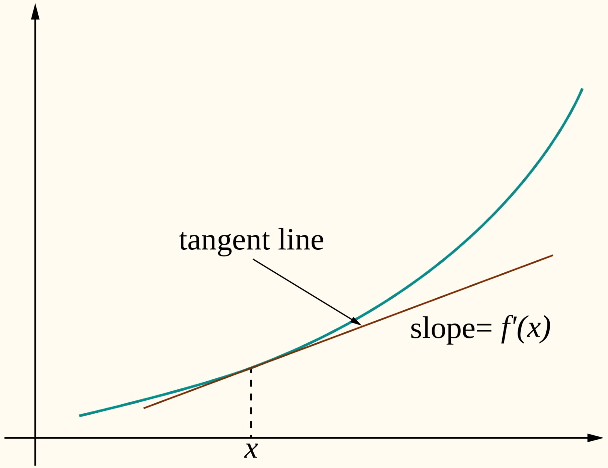
Derivatives (refresher)

Derivative at a point ***x*** is the slope of the tangent line on the function ***f***

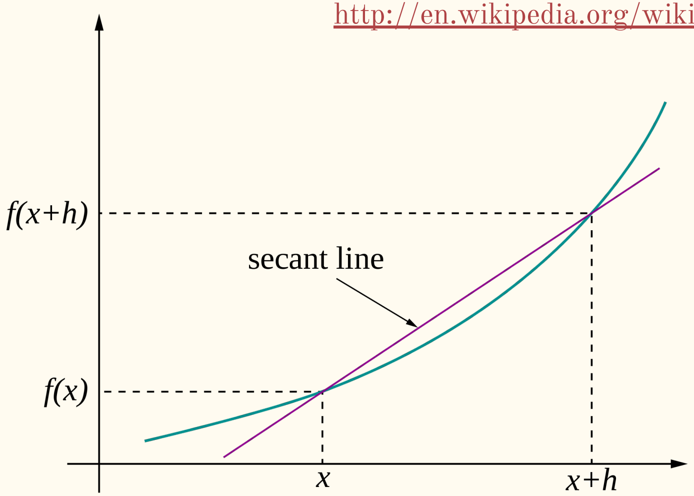
Best linear approximation of ***f*** near ***x***

Defined as this quotient:

$$\lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



http://en.wikipedia.org/wiki/Derivative



Taylor's theorem

For a function *f* that is continuously differentiable, there is *t* such that:

$$f(x+p) = f(x) + \nabla f(x+tp)p, t \in (0,1)$$

If twice differentiable:

$$f(x+p) = f(x) + \nabla f(x)p + \frac{1}{2}p\nabla^2 f(x+tp)p, t \in (0,1)$$

- We don't know ***t***, just that it exists
- Given value and gradients at ***x***, can approximate function at $\boldsymbol{x+p}$
- Higher degree gradients used, better approximation possible

Types of optimization algorithms

- Line search
- Trust region
- Gradient free
- Constrained optimization

Line search

At the current solution x_k, pick a **descent** direction first p_k, then find a stepsize α:

$$\min_{\alpha>0} f(x_k + \alpha p_k)$$

and calculate the next solution:

$$x_{k+1} = x_k + \alpha_k p_k$$

General definition of direction:

$$p_k = -B_k^{-1} \nabla f(x_k)$$

Gradient descent:

$$B_k = I$$

Newton method (assuming f twice differentiable and B_k invertible):

$$B_k = \nabla^2 f(x_k)$$

Gradient descent (for supervised MLE training)

Input: training examples $\mathcal{D} = \{(x^1, y^1), \ldots (x^M, y^M)\}$,
$learning\_rate\ \alpha$

Initialize weights w

while $\nabla_w NLL(w; \mathcal{D}) \neq 0$ **do**

Update $w = w - \alpha \nabla_w NLL(w; \mathcal{D})$

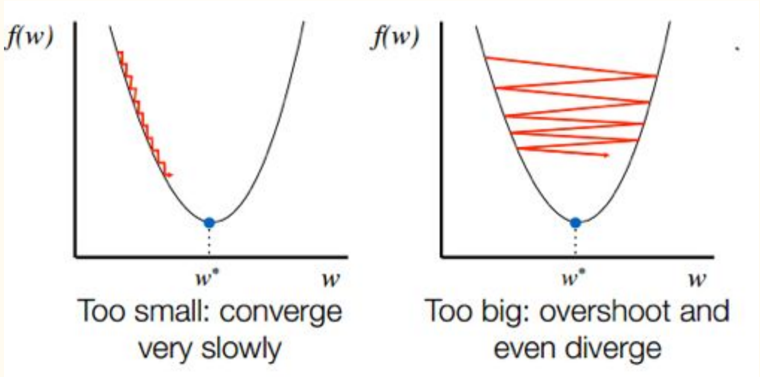
end while

To make it stochastic, just look at one training example in each iteration and go over each of them. Why is this a good idea?

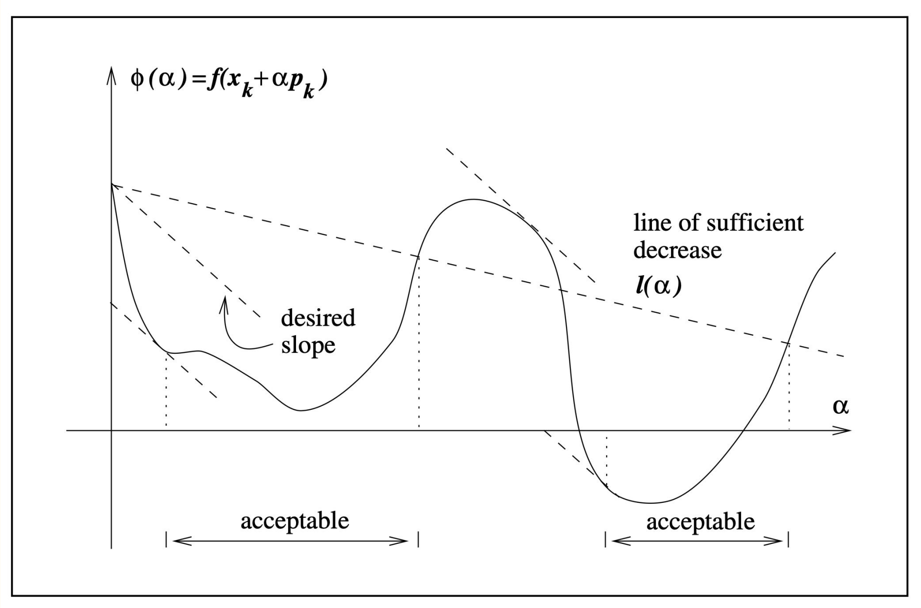
What can go wrong?

Gradient descent

Wrong step size:



https://srdas.github.io/DLBook/GradientDescentTechniques.html



Line search converges to the minimizer when the iterates follow the Wolfe conditions on sufficient decrease and curvature (Zoutendijk's theorem)

Back tracking: start with a large stepsize and reduce it to get sufficient decrease

Second order methods

Using the Hessian (line search Newton's method):

$$x_{k+1} = x_k - \alpha_k \nabla^2 f(x_k)^{-1} \nabla f(x_k)$$

Expensive to compute. Can we approximate?

Yes, based on the first order gradients:

$$B_{k+1} = \frac{\nabla f(x_{k+1}) - \nabla f(x_k)}{x_{k+1} - x_k}$$

BFGS calculates B_{k+1}^{-1} directly without moving too far from B_k^{-1}

What are desirable properties in line search?

Fast convergence:

- Few iterations
  - Stochastic gradient descent will have more than standard gradient descent
- Cheap iterations; what makes them expensive?
  - Function evaluations for backtracking with line search (this is the reason for researching adaptive learning rates)
  - (approximate) second order gradients (partly why they are not used in DL)

Memory requirements? Storing second order gradients requires $|w|^2$. One of the key variants of BFGS is L(imited memory)-BFGS.

One can learn the updates: Learning to learn gradient descent by gradient descent

Trust region

Taylor's theorem:

$$f(x+p) = f(x) + \nabla f(x)p + \frac{1}{2}p\nabla^2 f(x+tp)p, t \in (0,1)$$

Assuming an approximation m to the function f we are minimizing:

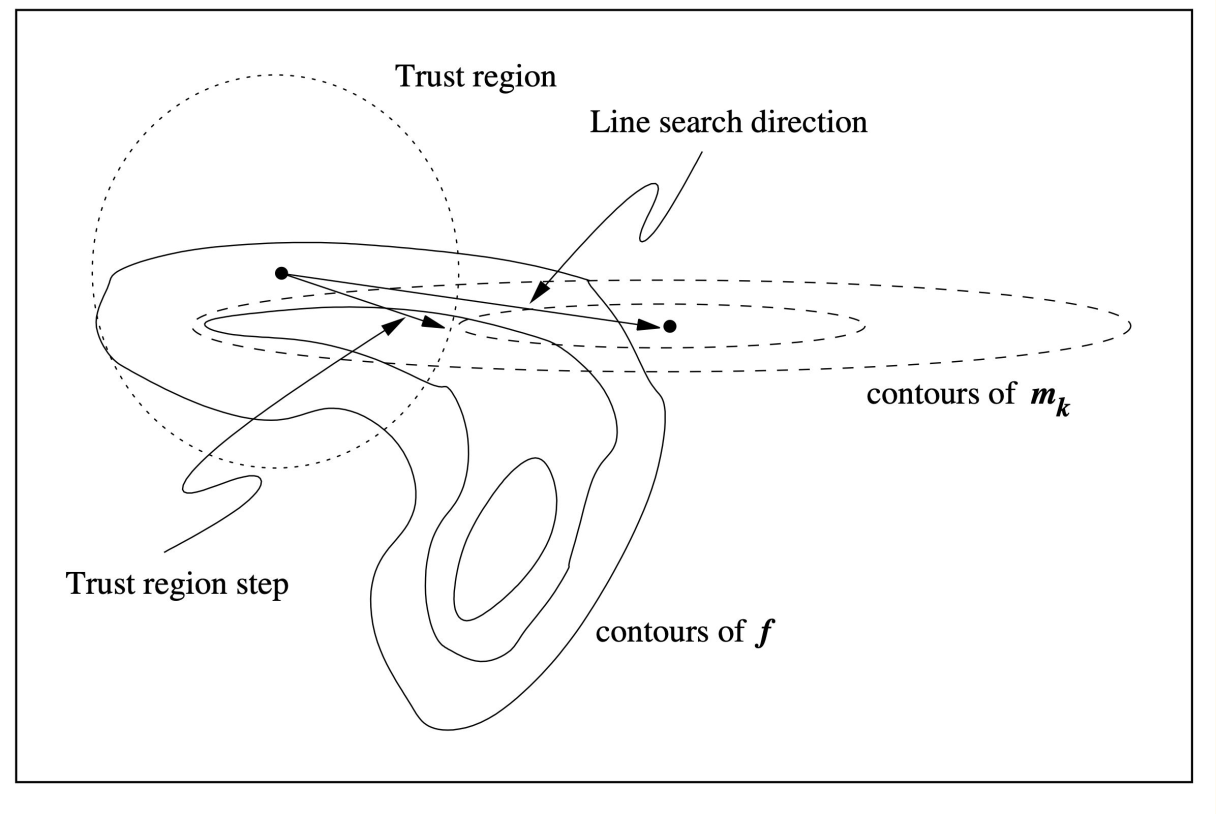
$$m_k(p) = f(x_k) + \nabla f(x_k)p + \frac{1}{2}p\nabla^2 f(x_k)p$$

Given a radius Δ (max stepsize, **trust region**), choose a direction p such that:

$$\min_p m_k(p), p \leq \Delta_k$$

Measuring trust: $$\frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}$$

Trust region



Worth considering with relatively few dimensions.

Recent success in [reinforcement learning]

Gradient free

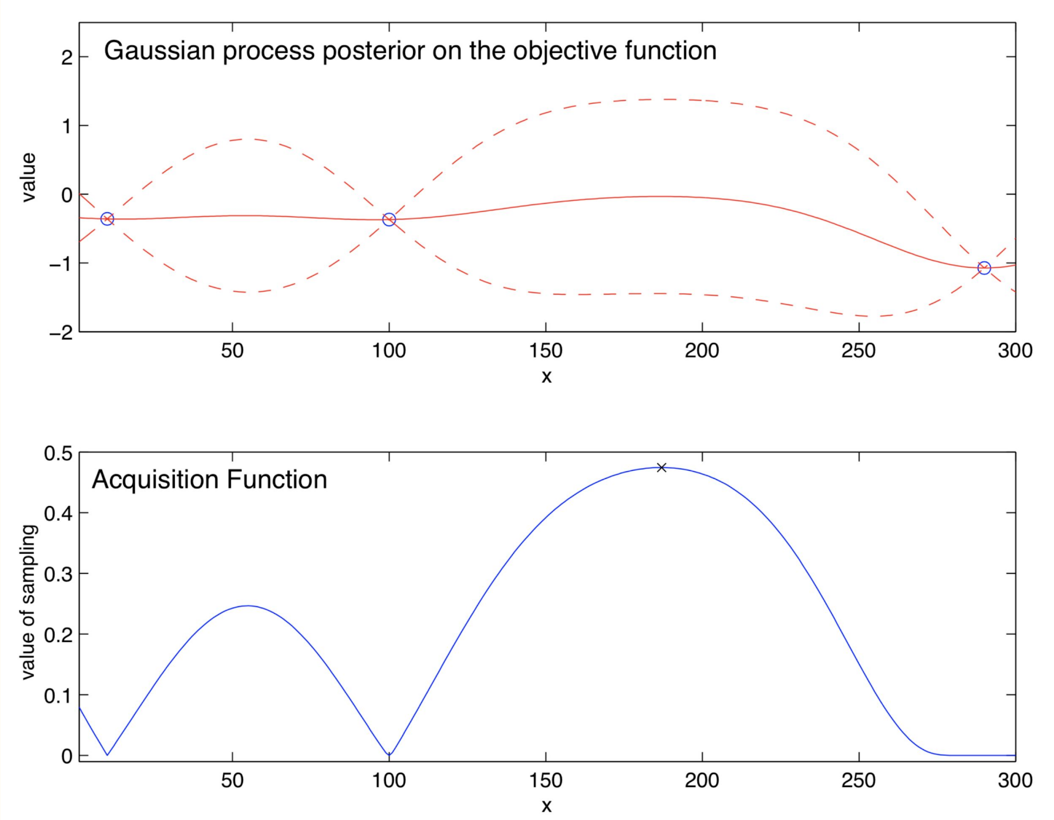
What if we don’t have/want gradients?

- Function is a black box to us, can only test values
- Gradients too expensive/complicated to calculate, e.g.: hyperparameter optimization

Two large families:

- Model-based (similar to trust region but without gradients for the approximation model)
- Sampling solutions according to some heuristic
    - Nelder-Mead
    - Evolutionary/genetic algorithms, particle swarm optimization

Bayesian Optimization



- Model approximation based on Gaussian Process regression
- Acquisition function tells us where to sample next
- See here for a nice illustration

Frazier (2018)

Constraints

Reminder: $$x^\star = \arg\min_x f(x), c(x) \geq 0$$

Minimizing the Lagrangian function converts it to unconstrained optimization (for equality constraints, for inequalities it is slightly more involved):

$$L(x, \lambda) = f(x) - \lambda c(x)$$

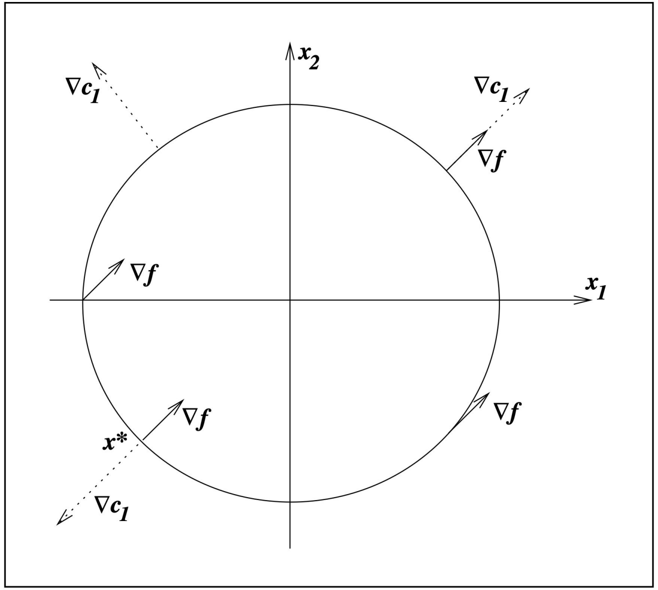
$$\nabla L(x, \lambda) = 0 \Rightarrow \nabla f(x^\star) = \lambda^\star \nabla c(x^\star)$$

Intuition: the gradients at min/max are parallel

Example:

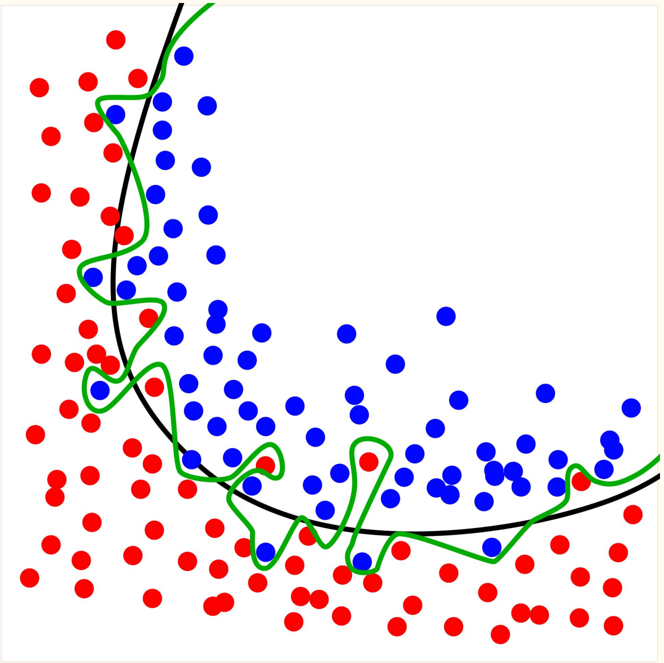
$$f(x_1, x_2) = x_1 + x_2$$

$$c(x_1, x_2) = x_1^2 + x_2^2 - 2 = 0$$

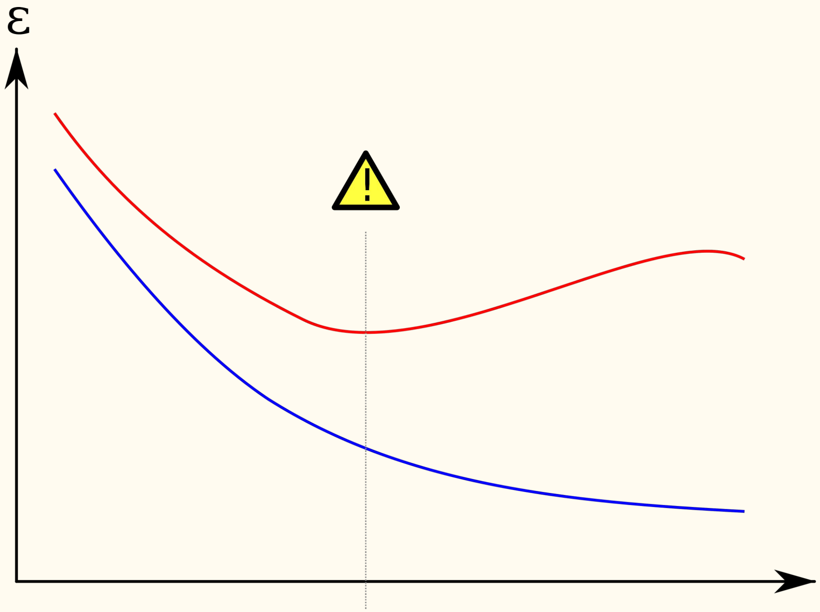


Overfitting

Separating hyperplanes in training



Error during training and testing



https://en.wikipedia.org/wiki/Overfitting#Machine_learning

Regularization

We want to optimize the function/fit the data but not too much:

$$w^\star = \arg\min_w L(w; \mathcal{D}) + \lambda \mathcal{R}(w)$$

Some options for the regularizer:

- L2 (ridge): Σw^2
- L1 (Lasso): $\Sigma |w|$
- Elastic net: L1+L2
- L-infinity: $\max(w)$

Words of caution

Sometimes we are saved from overfitting by not optimizing well enough

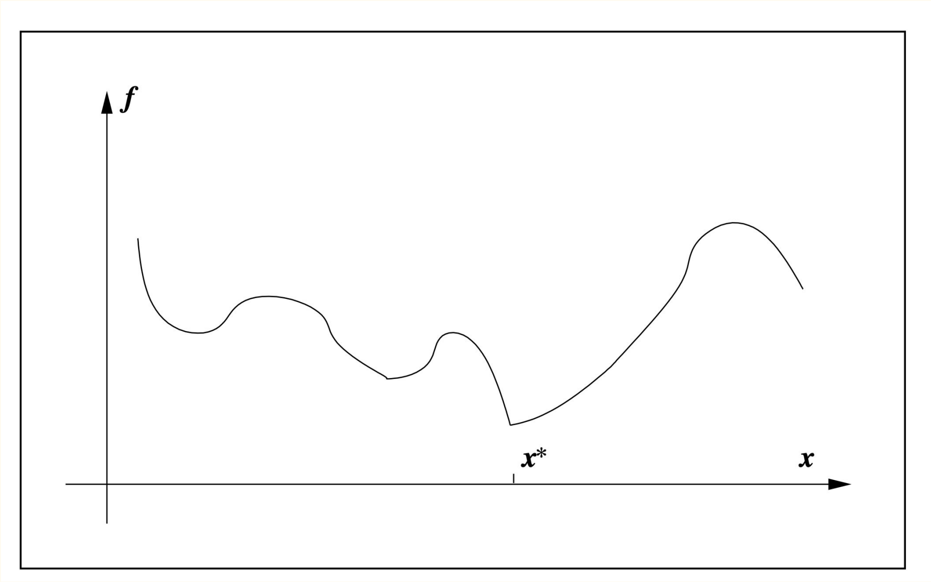
There is often a discrepancy between loss and evaluation objective; often the latter are not differentiable (e.g. BLEU scores)

Check your objective if it tells you the right thing: optimizing less precisely and getting better generalization is OK, having to optimize badly to get results is not.

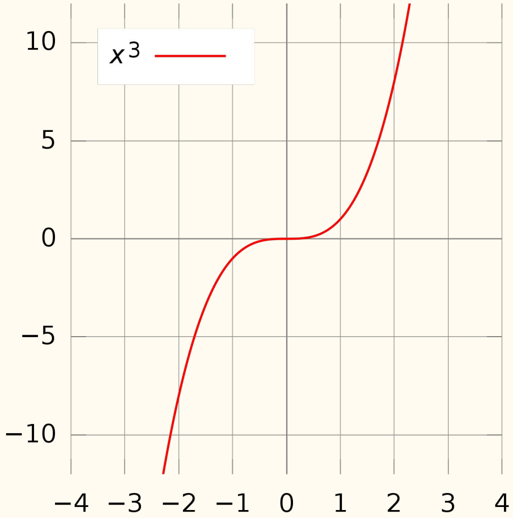
Construct toy problems: if you have a good initial set of weights, does optimizing the objective leave them unchanged?

Harder cases

- Non-convex
- Non-smooth



Saddle points: zero gradient is a first order **necessary condition, not sufficient**



https://en.wikipedia.org/wiki/Saddle_point

Bibliography

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- On integer (linear) programming in NLP: https://ilpinference.github.io/eacl2017/
- Francisco Orabona's blog: https://parameterfree.com
- Dan Klein's Lagrange Multipliers without Permanent Scarring
- A course on optimization in ML by Roger Grosse: https://www.cs.toronto.edu/~rgrosse/courses/csc2541_2022/