Deep Learning (BEV033DLE)
Lecture 8
Adaptive SGD Methods

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- Geometry of Neural Network Loss Surfaces
  - Local Minima and Saddle Points in nD
  - Parameter redundancy helps optimization
- Understanding Adaptive Methods
  - Proximal Problems, Convex vs non-convex, Stochastic optimization
  - Adam, RMSprop, Adargad
- Examples of Changing the Space Metric
  - Change of Coordinates, Preconditioning, Equivalent reparameterizations, Constraints

Loss Landscape

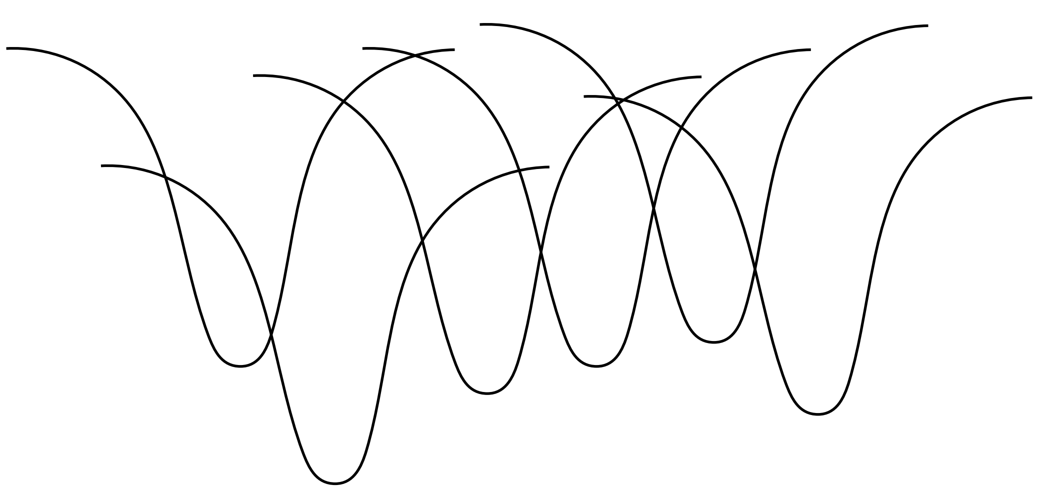
Local Minima

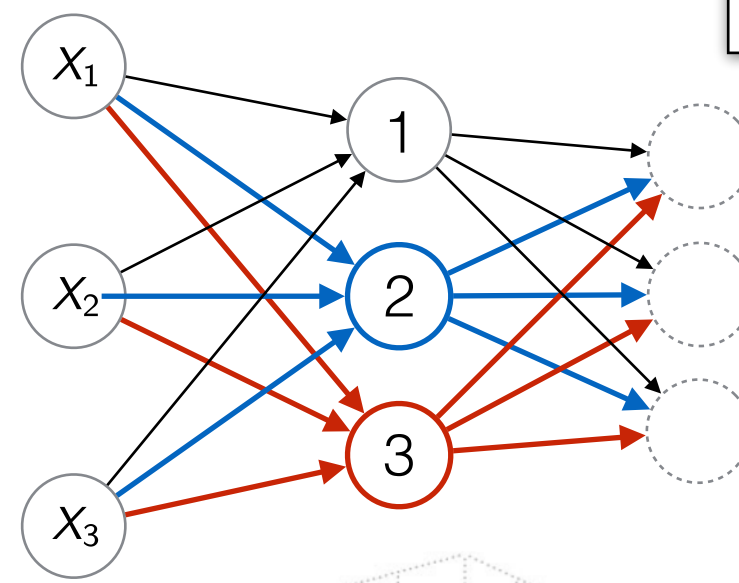
✦ There are several reasons for local minima

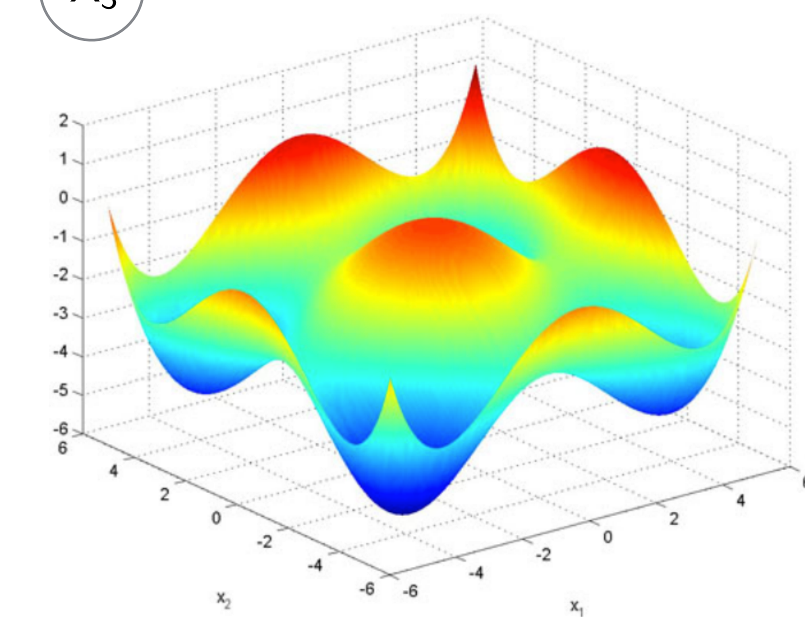
- **Symmetries** (Permutation invariances)
  - Fully connected layer with **n** hidden units: **n!** permutations
  - Convolutional layer with **c** channels: **c!** permutations
  - In a deep network many equivalent local minima, but all of them are equally good -- no need to avoid
- Loss function is a **sum of many non-convex terms**:

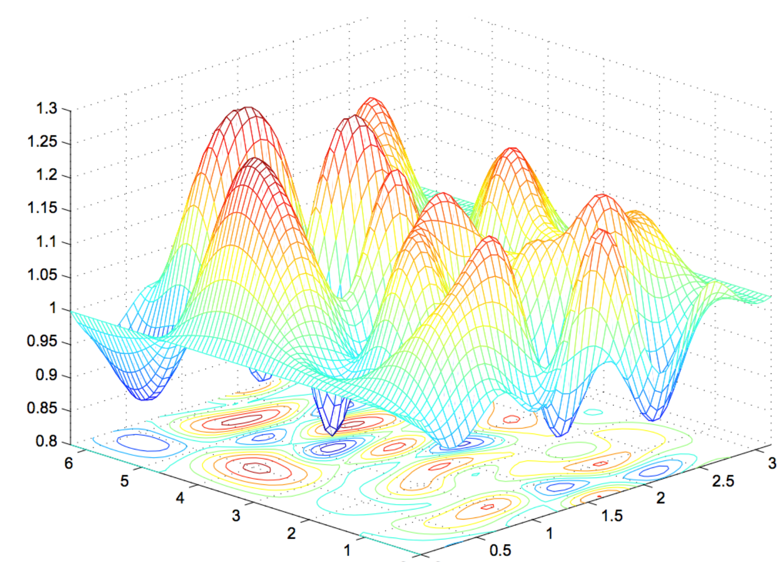
$$L(\theta) = \sum_i l(y_i, f(x_i; \theta))$$

often convex — non-linear



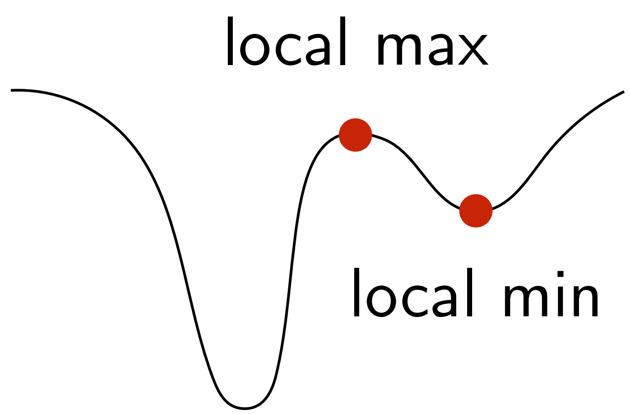




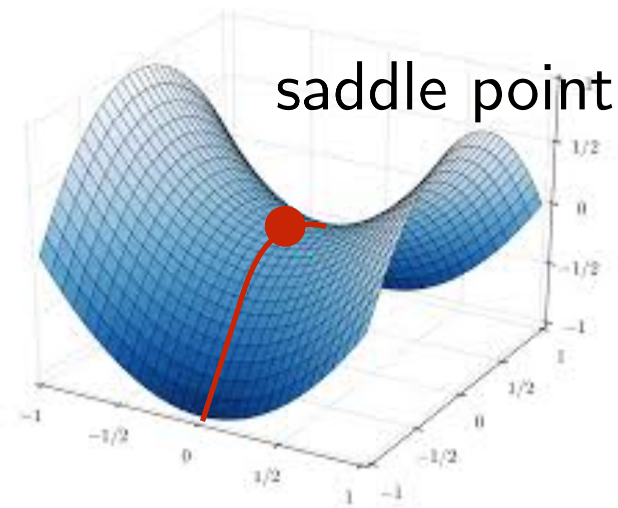


Local Minima in High Dimensions

1D



2D



- local min in one dimension
- it is still possible to descend in other dimension
- but can be getting stuck

nD

Let $f(x+\Delta x) \approx f(x) + J\Delta x + \Delta x^{\mathsf{T}} H \Delta x$,

where H has eigenvalues $\lambda_1, \dots \lambda_2$.

Important characteristic (**index**): α — the fraction of negative eigenvalues.

A point x is

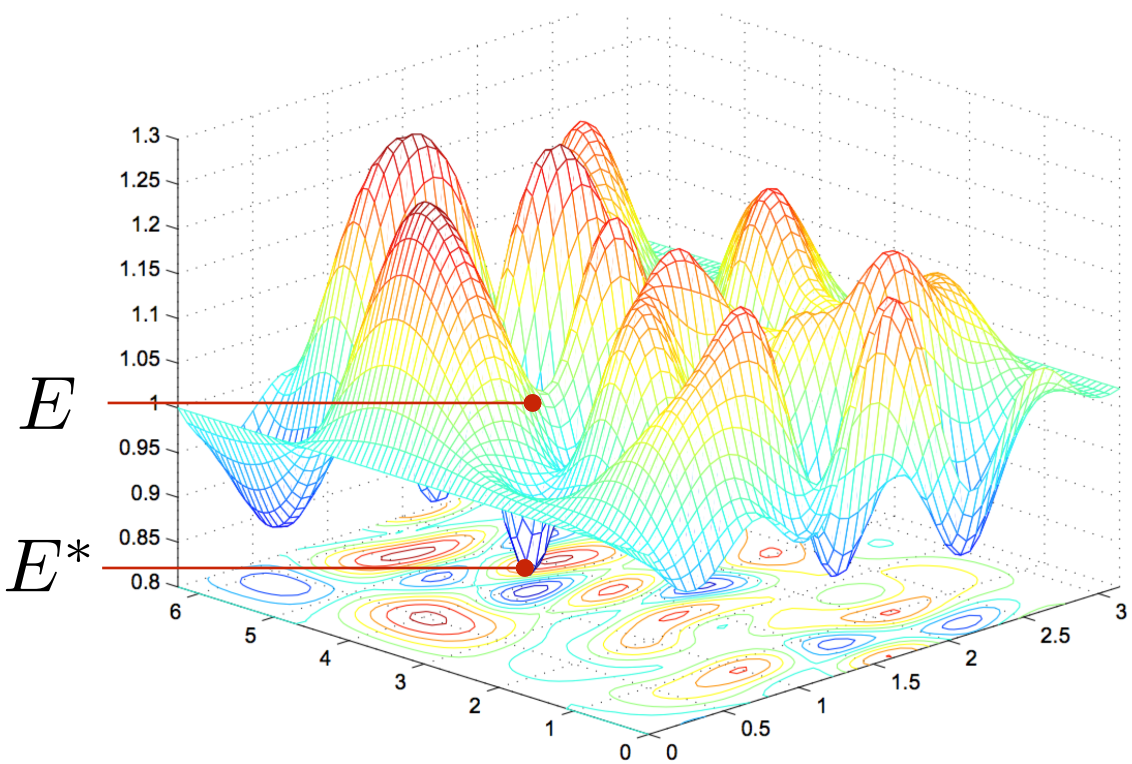
A **Stationary** if the gradient at x is zero

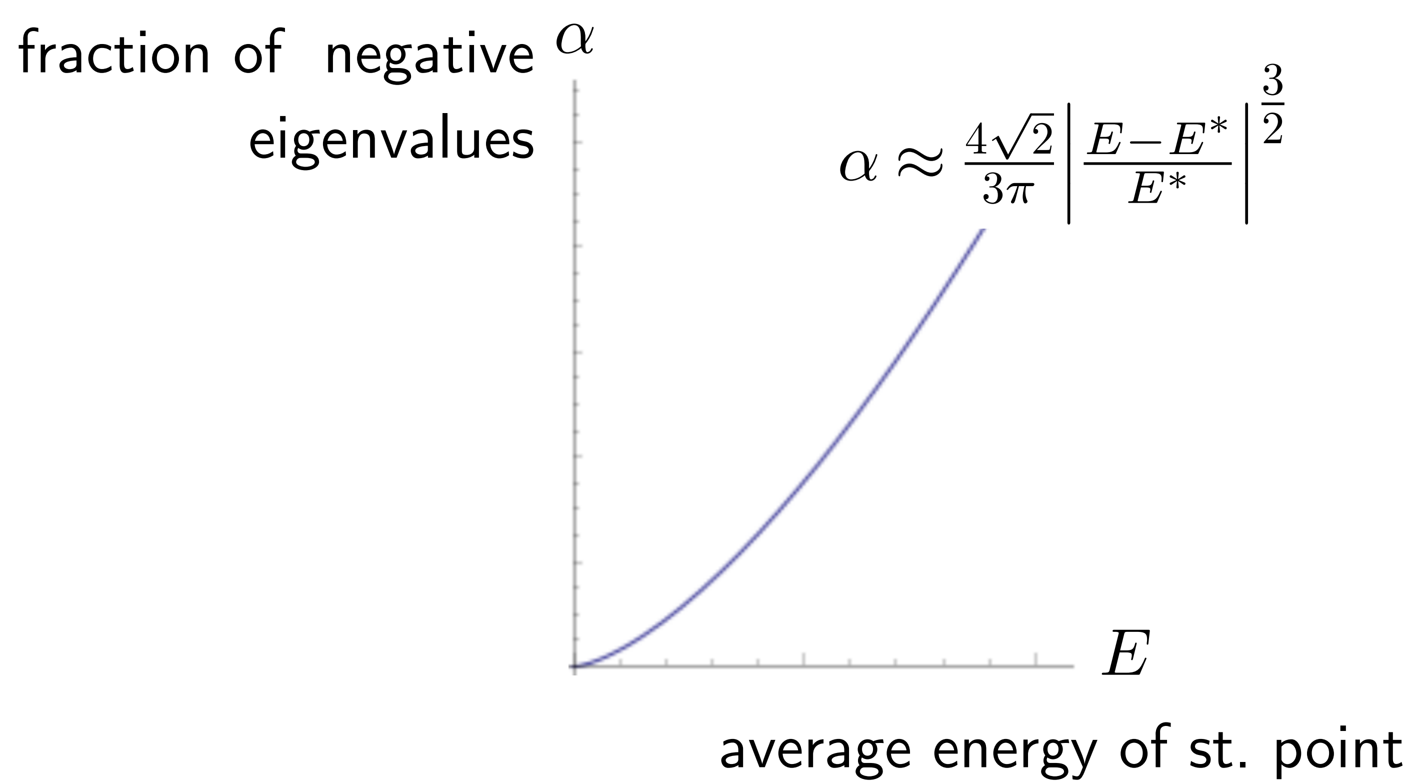
A **Saddle**: if it is stationary and $0 < \alpha < 1$

A **Local minnimum**: if it is stationary and $\alpha = 0$.

Local Minima in High Dimensions

- Insights from Theoretical Physics --- **Gaussian Fields**:
  - local minima are exponentially more rare than saddle points
  - they become likely at lower energies (loss values)

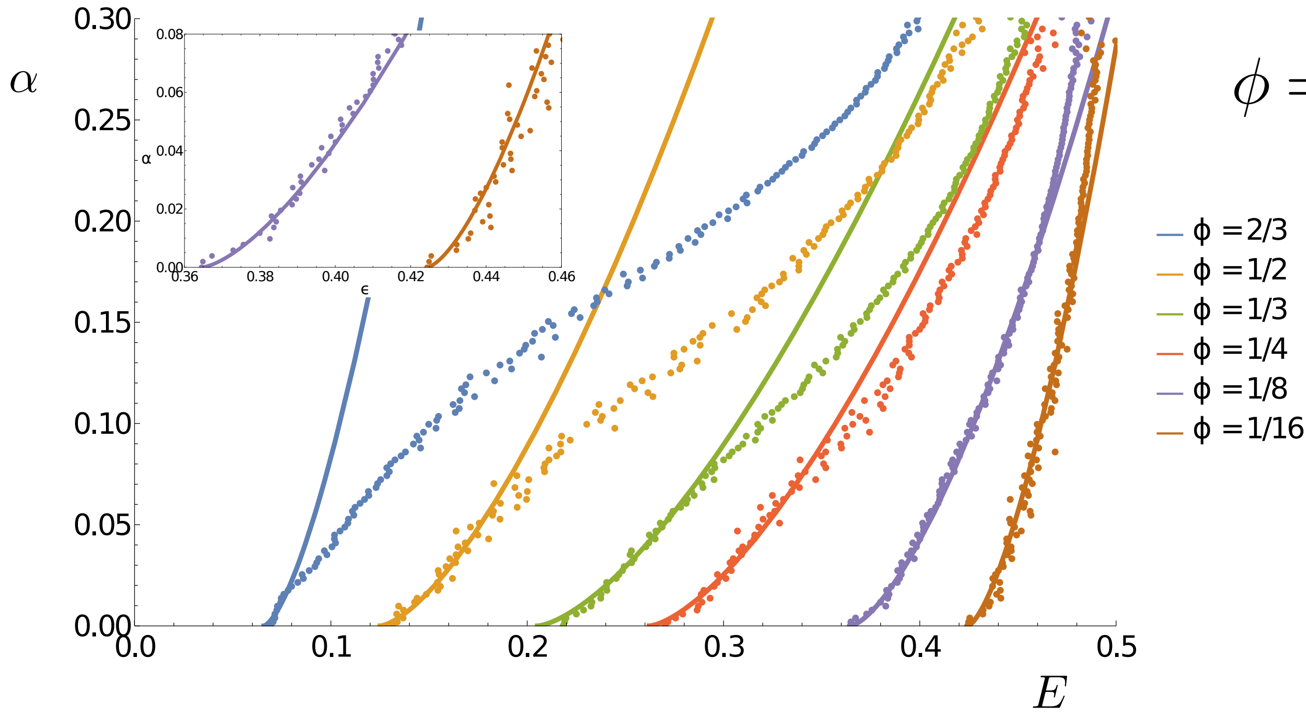




[Bray & Dean (2007) The statistics of critical points of Gaussian fields on large-dimensional spaces]

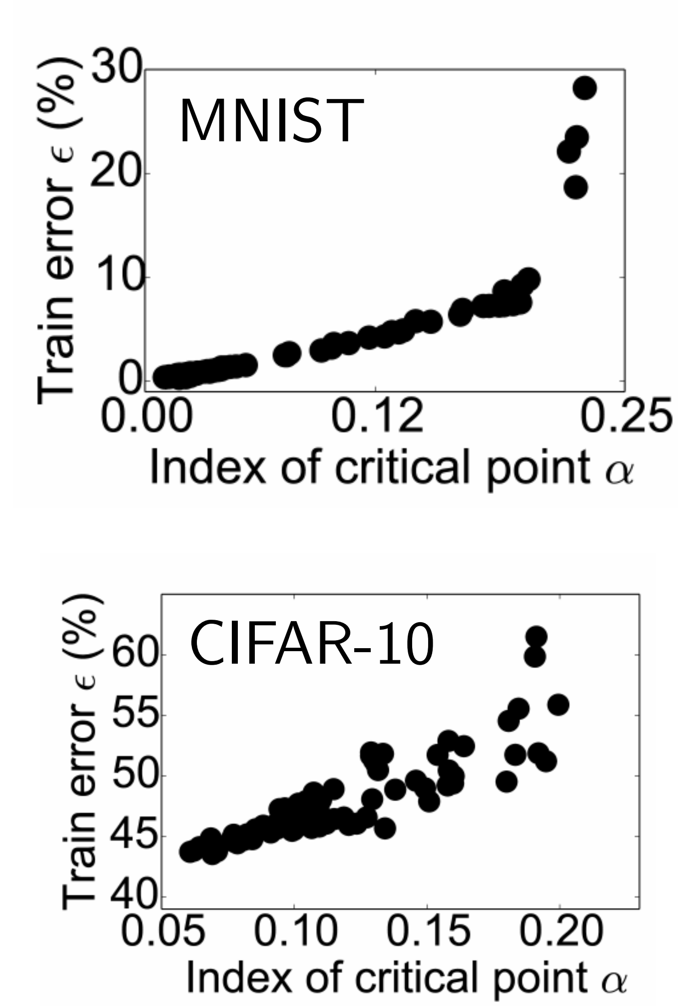
Local Minima in High Dimensions

✦ Experimental Confirmations in Neural Networks



$$\phi = \frac{\#\text{parameters}}{\#\text{samples}}$$

[Pennington & Bahri 2017]



[Dauphin et. al. 2017]

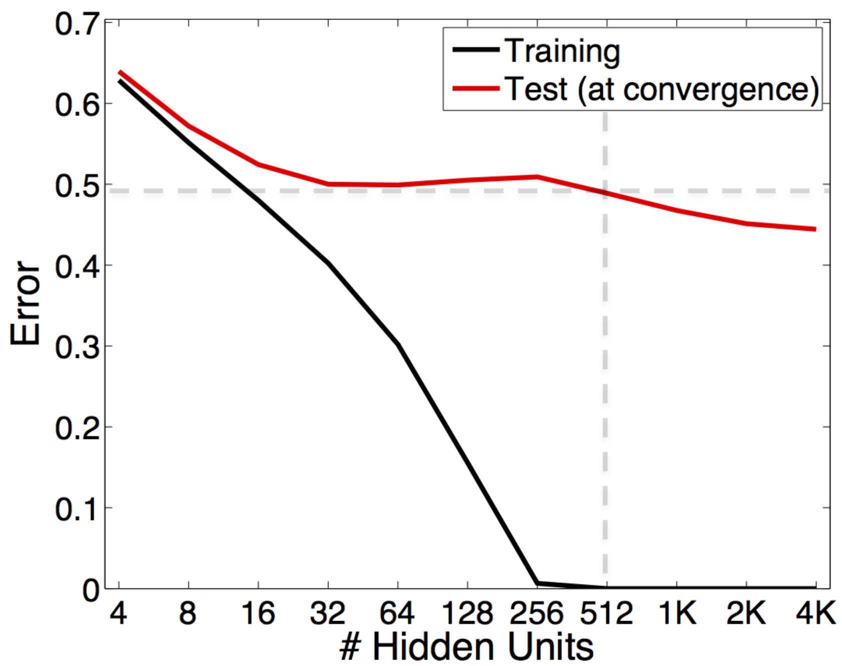
- 1 hidden layer
- good agreement for small alpha (as expected)

[Pennington & Bahri (2017) Geometry of Neural Network Loss Surfaces via Random Matrix Theory]

[Dauphin et. al. (2017) Identifying and attacking the saddle point problem in high-dimensional non-convex optimization]

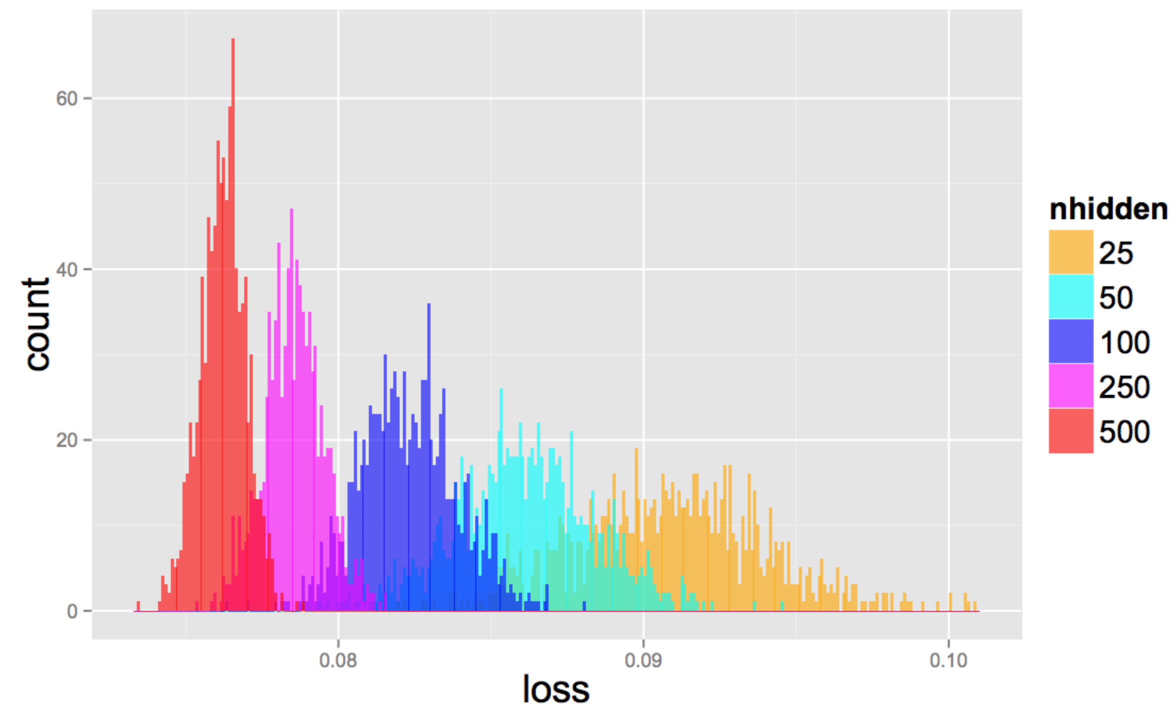
High Dimensionality Helps Optimization

Achieve 0 training error
with sufficiently large networks



[Neyshabur (2015)]

Histogram of SGD trials



[Choromanska et al. (2015):
The Loss Surfaces of Multilayer Networks]

✦ **Summary**:

- Local minima are rare and appear to be good enough
  (note, we just waved an NP-hard non-convex optimization problem)
- But we need (highly) overparametrized models to have this easy training
- We hope that overparametrized models will still generalize well
- Maybe, optimization should worry a bit about efficiency around saddle points

Adaptive Methods

Need for Adaptive Methods

- In deep models we have:
  - **different kinds** of parameters: weights, biases, normalization parameters
  - located in **different layers**
  - Some parameters may be more sensitive than other
  - Some directions in the parameter space may be more sensitive (e.g. due to high curvature)
- Gradient Step Depends on the Choice of Coordinates
  - It is not necessarily the best direction for a step

- Many adaptive methods have emerged:

RMSProp	VAdam	Adamax
Adagrad	PAdam	AmsGrad
AdaDelta	Nadam	Yogi
Adam	AdamW	...
BAdam	AdamX	

Common Adaptive Methods

- **Adagrad**:

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\varepsilon}{\sqrt{t}} \frac{\tilde{g}_{t,i}}{\sqrt{\text{Mean}\left(\tilde{g}^2_{1:t,i}\right)}}$$

- **RMSProp**:

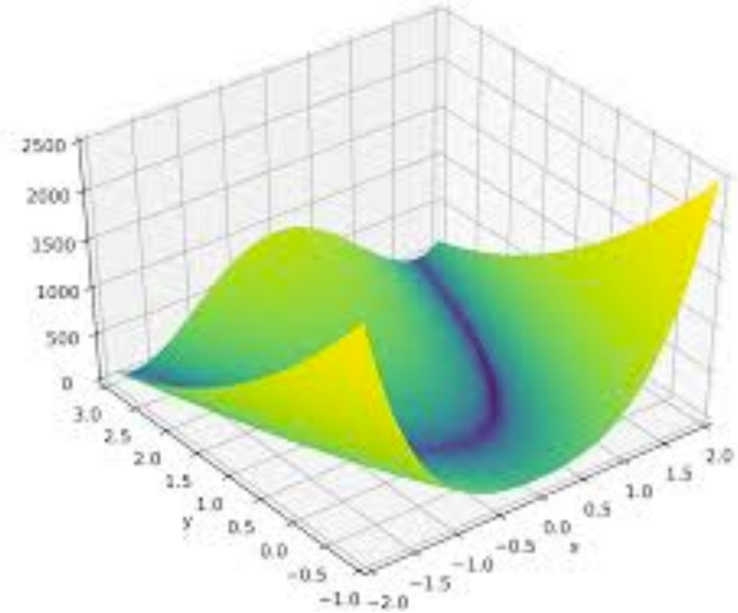
$$\theta_{t+1,i} = \theta_{t,i} - \varepsilon \frac{\tilde{g}_{t,i}}{\sqrt{\text{EWA}\left(\tilde{g}^2_{1:t,i}\right)}}$$

- **Adam**:

$$\theta_{t+1,i} = \theta_{t,i} - \varepsilon \frac{\text{EWA}_{\beta_1}\left(\tilde{g}_{1:t,i}\right)}{\sqrt{\text{EWA}_{\beta_2}\left(\tilde{g}^2_{1:t,i}\right)}}$$

- All updates work per coordinate i independently
- $\tilde{g}_{1:t,i}$ denotes the sequence of all past gradients
- They are adaptive because each coordinate is rescaled differently
- Mostly differ by running averages used

- While they do work better for functions with valleys, explaining them as second order methods has quite some gaps
- This lecture:
  - consider some general useful optimization ideas
  - that (hopefully) will provide insights for this design as well



Proximal Problem and Trust Region

- Let's revisit how do we find the step Δx for SGD
  - Linearize: $f(x_0 + \Delta x) \approx f(x_0) + J\Delta x$
  - Trust this approximation only for $\|\Delta x\| \le \varepsilon$
  - **Step proximal problem**:

$$\min_{\|\Delta x\| \le \varepsilon} \left(f(x_0) + J\Delta x\right)$$

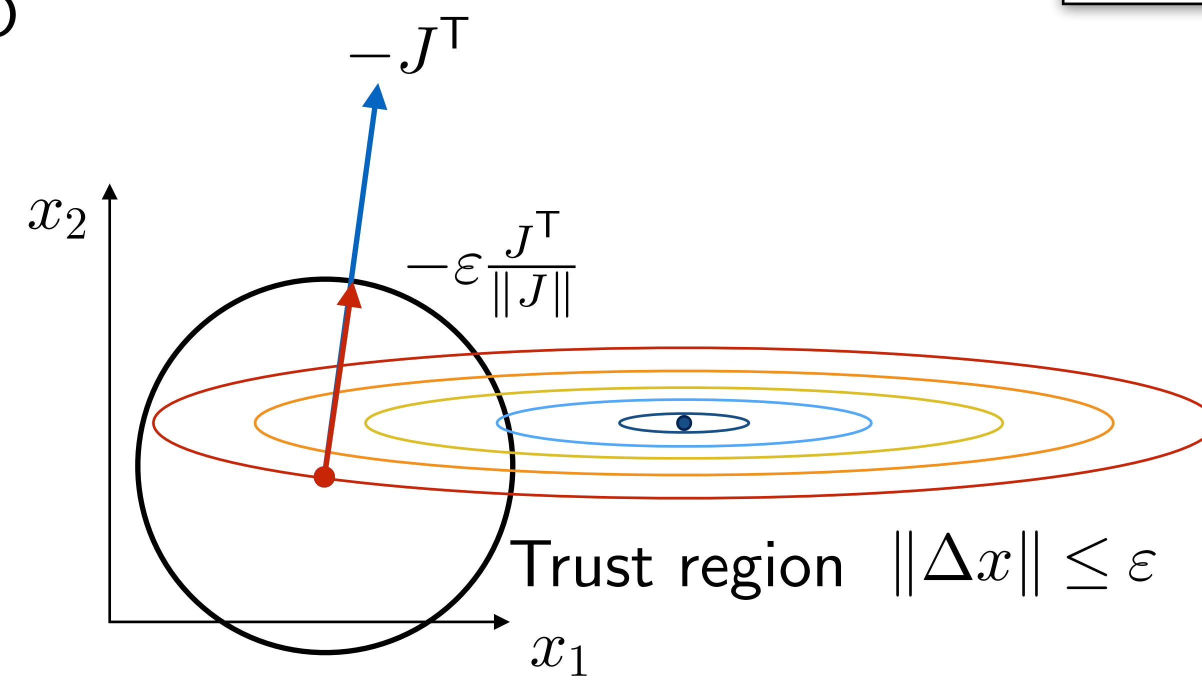
Equivalent to:

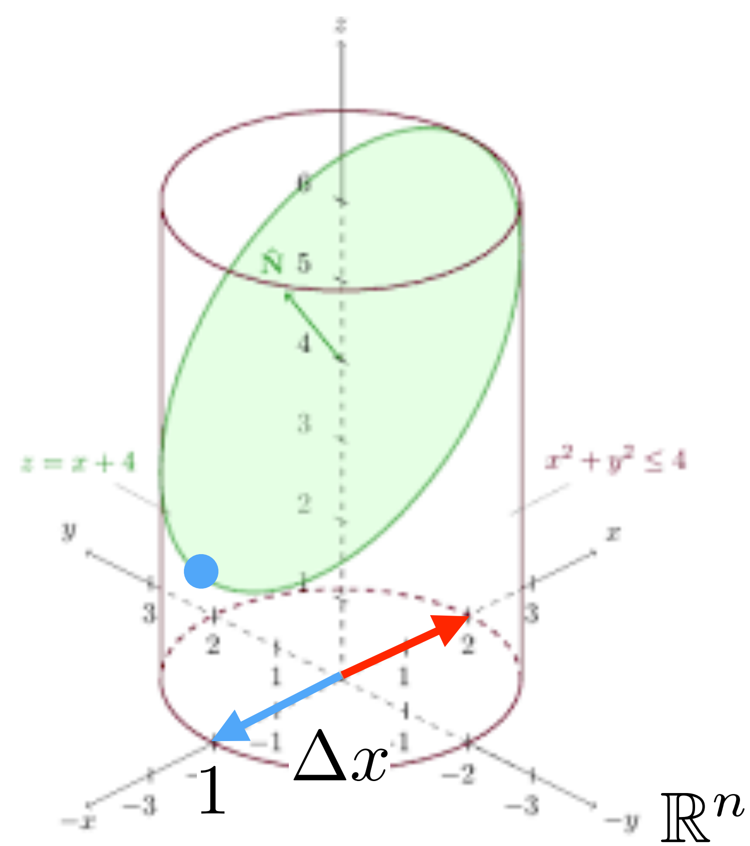
$$\max_{\lambda} \min_{\Delta x} \left(J\Delta x + \lambda(\|\Delta x\|^2 - \varepsilon^2)\right)$$

Step direction: $\Delta x = -\frac{1}{2\lambda} J^\mathsf{T}$

$\|\Delta x^\mathsf{T}\|^2 = \varepsilon^2 \to \lambda = \frac{1}{2\varepsilon}\|J\|$

Trust region step: $\Delta x = -\varepsilon \frac{J^\mathsf{T}}{\|J\|}$

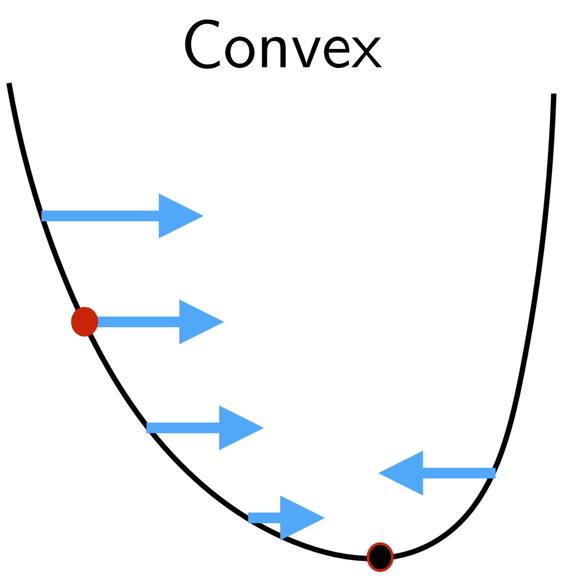




- Generates two kinds of steps:
  - Proportional to gradient length (SGD)
  - Using only gradient direction (normalize)
- We can choose trust regions differently

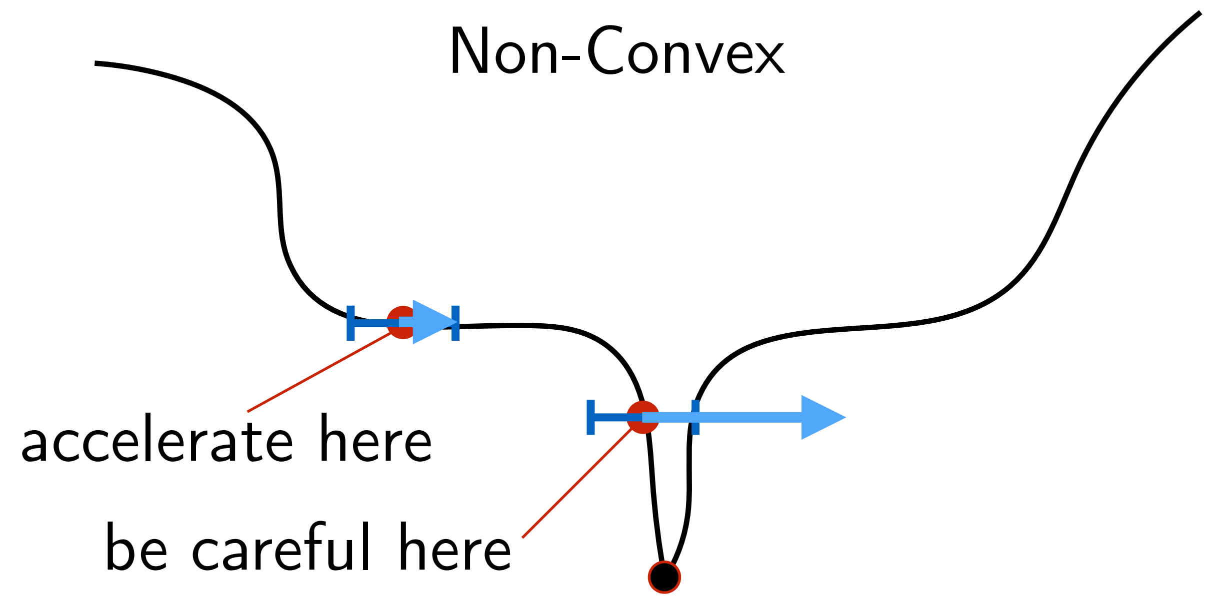
Differences of Convex vs. Non-Convex

<u>Why to step proportional to the gradient:</u>



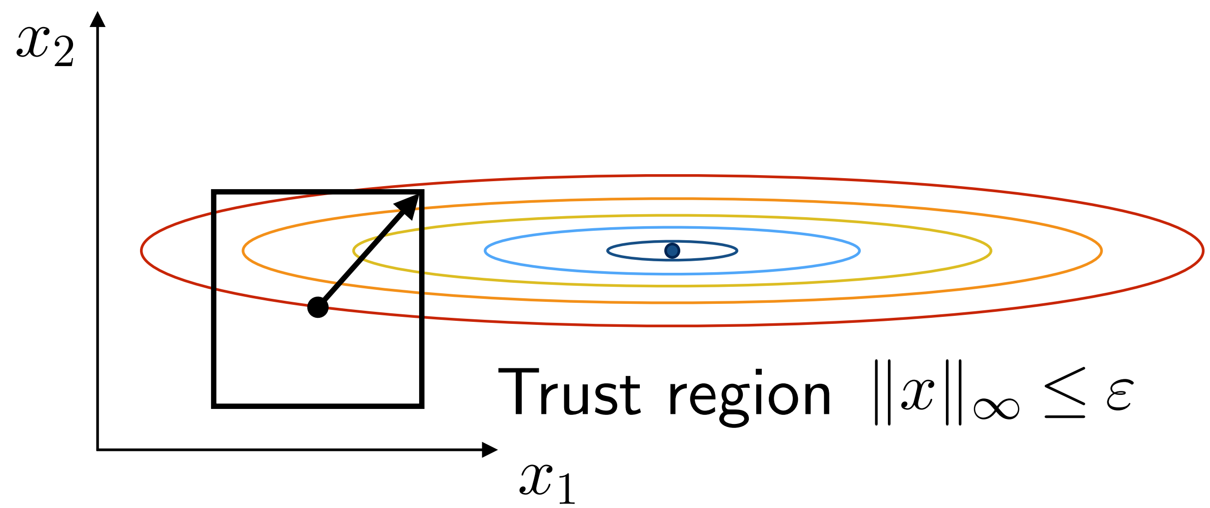
- No other stationary points than global minima
- **The further we are from the optimum, the larger is the gradient**: $\exists \mu > 0$
  - $\|\nabla f(x)\|^2 \geq \mu(f(x) - f^*)$
  - $\|\nabla f(x)\| \geq \mu|x - x^*|$
- Negative gradient points towards the optimum:
  - $\langle -\nabla f, x^* - x \rangle \geq f - f^* + \tilde{\mu}\|x - x^*\|^2$
  - Optimization need not be monotone in f

<u>Why to normalize:</u>



- Gradient carries no global information
  - Need bigger steps where gradient and curvature are low
  - Need smaller steps when gradient and curvature are high
- Makes sense to use **trust region steps**:
  - $\Delta x = -\frac{\nabla f}{\|\nabla f\|}$
  - If the trust region is ok, should guarantee a steady progress

Box Trust Regions



- This time solve for step as:
  - $\min_{\|\Delta x_i\| \le \varepsilon \ \forall i} \left(f(x_0) + J\Delta x \right)$
    (In overparametrized models expect many parameters to have independent effect)
  - Equivalent to:

    $$\max_{\lambda} \min_{\Delta x} \left(J\Delta x + \sum_i \lambda_i (\|\Delta x_i\|^2 - \varepsilon^2) \right)$$

    $$2\lambda_i \Delta x_i = -J_i$$

    Step direction: $\Delta x_i = -\frac{1}{2\lambda_i} (\nabla f(x))_i$

    Trust region step: $\Delta x_i = -\varepsilon \frac{(\nabla f(x))_i}{\|(\nabla f(x))_i\|}$

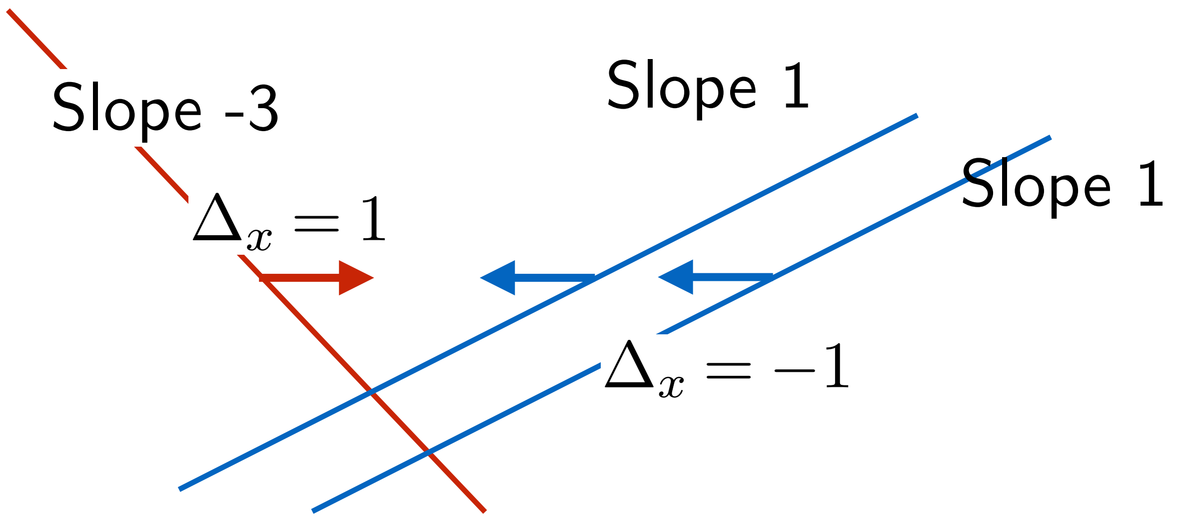
Non-Convex Stochastic

- Trust region steps: $\Delta x = -\frac{\nabla f(x)}{\|\nabla f(x)\|}$
- Problem: breaks in the stochastic setting
- Example

  $f(x) = (-3x) + (x) + (x+1)$, chose 1 summand at a time with equal probability

  If we normalize stochastic gradients,

  will move in the wrong direction!



- Want the steps to follow the descent direction on average
  - Cannot adjust the stochastic gradient "too much nonlinearly"

Non-Convex Stochastic

- **Solution**: use running averages to approximate the expectation form:

  $\Delta x = -\varepsilon \frac{\mathbb{E}[\nabla f]}{\|\mathbb{E}[\nabla f]\|}$

  Also note that $\|\mathbb{E}[\nabla f]\| = \sqrt{(E[\nabla f])^2} \leq \sqrt{(E[(\nabla f)^2])}$

  – may be interpreted as a more robust setting

- **Adagrad**:

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\varepsilon}{\sqrt{t}} \frac{\tilde{g}_{t,i}}{\sqrt{\text{Mean}\left(\tilde{g}^2_{1:t,i}\right)}}$$

- **RMSProp**:

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- **Adam**:

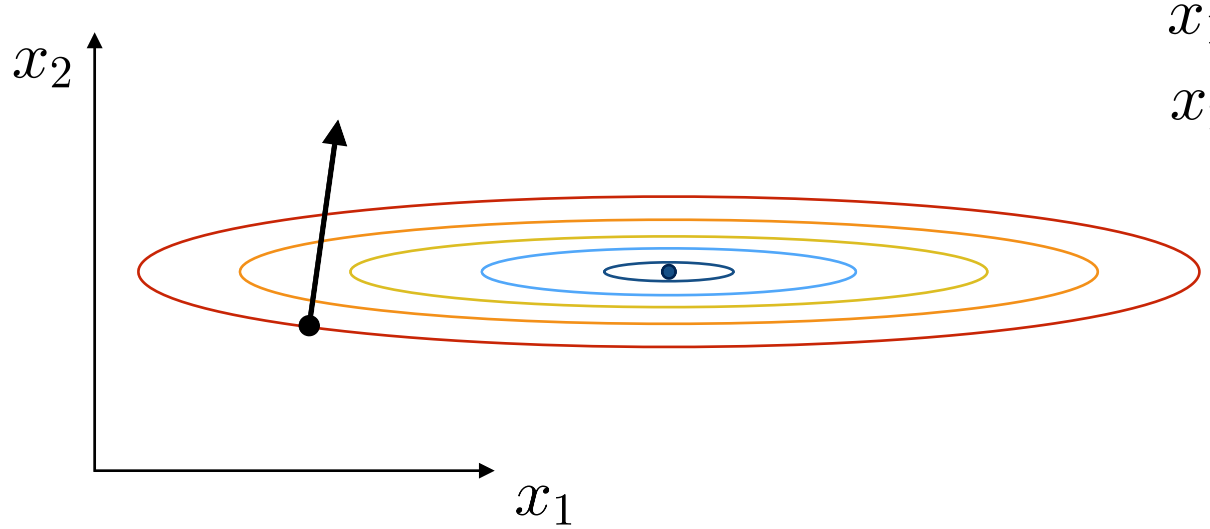
$$\theta_{t+1,i} = \theta_{t,i} - \varepsilon \frac{\text{EWA}_{\beta_1}\left(\tilde{g}_{1:t,i}\right)}{\sqrt{\text{EWA}_{\beta_2}\left(\tilde{g}^2_{1:t,i}\right)}}$$

- In Adagrad:
  $\frac{1}{\sqrt{t}}$ guarantees convergence
- Other methods would also need this in theory but are typically presented and used with constant ε
  For sparse gradients, $t\,\text{Mean}(\tilde{g}^2_{1:t,i})$ could grow much slower than t and achieve a speed-up compared to SGD
- In Adam:
  EWA with $\beta_1 = 0.9$ works as common momentum (20 batches averaging)
  EWA with $\beta_2 = 0.999$ (2000 batches averaging) makes the normalization smooth enough

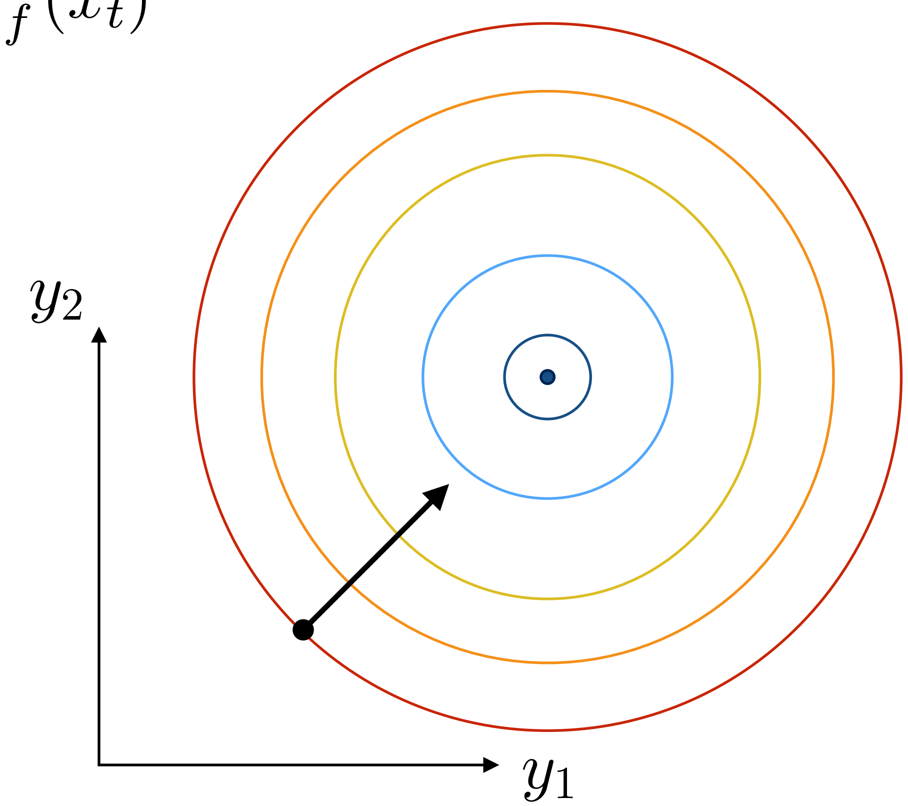
More Examples of Changing the Metric

Gradient Depends on the Choice of Coordinates

- Consider the simple gradient descent for a function $f\colon \mathbb{R}^n \to \mathbb{R}$:
  - $\min_{x\in\mathbb{R}^n} f(x)$
  - $x_{t+1} = x_t - \alpha J_f^{\mathsf{T}}(x)$
- Make a substitution: $x = Ay$ (change of coordinate) and write GD in y:
  - $\min_{y\in\mathbb{R}^n} f(Ay)$
  - $y_{t+1} = y_t - \alpha A^{\mathsf{T}} J_f^{\mathsf{T}}(Ay_t)$
- Substitute back $y = A^{-1}x$:
  - $A^{-1}x_{t+1} = A^{-1}x_t - \alpha A^{\mathsf{T}} J_f^{\mathsf{T}}(x_t)$
  - Obtained **preconditioned** GD: $x_{t+1} = x_t - \alpha(AA^{\mathsf{T}}) J_f^{\mathsf{T}}(x_t)$
  - $P = AA^{\mathsf{T}}$ – positive semidefinite
  - $P\nabla f(x)$ – is a descent direction



$x_1 = y_1$
$x_2 = 5y_2$



- Similar for non-linear change of coordinates, e.g. normalization

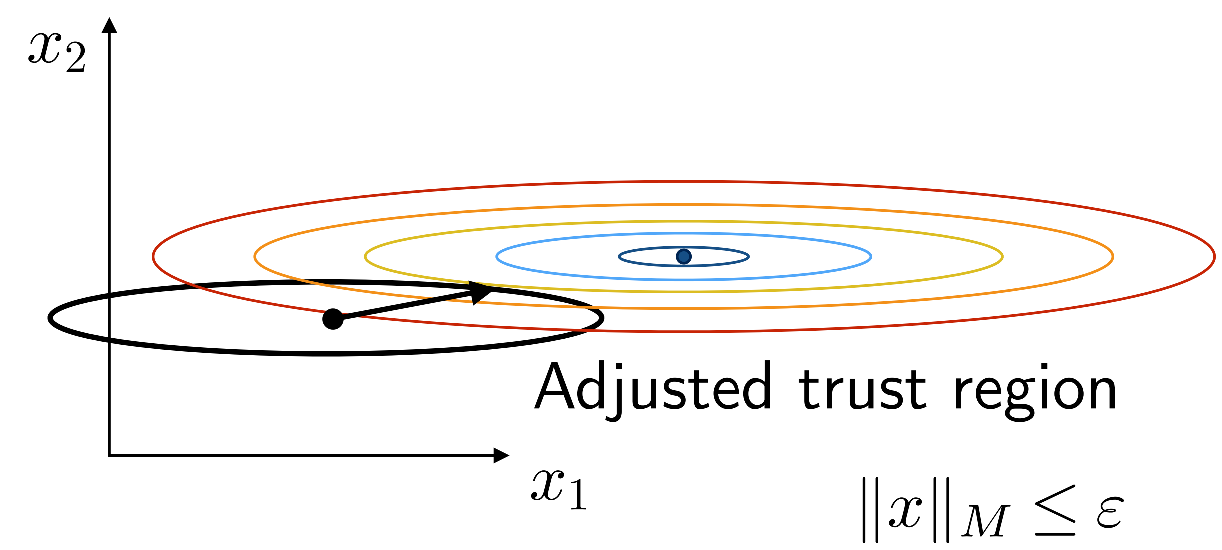
Mahalanobis Metric

- Adjust the trust region for sensitivity in different parameters:
  - $\min_{\|\Delta x\|_M \leq \varepsilon} \big(f(x_0) + J\Delta x\big)$ for given ε
  - $\|\Delta x\|_M = (\Delta x^\mathsf{T} M \Delta x)^{\frac{1}{2}}$ – Mahalanobis distance

  Equivalent to:

  $$\max_{\lambda} \min_{\Delta x} \Big(J\Delta x + \lambda(\|\Delta x\|_M^2 - \varepsilon^2)\Big)$$

  Step direction: $\Delta x = -\frac{1}{2\lambda} M^{-1} \nabla f(x)$



- Intuitive way to understand preconditioning
  - Can associate sensitivity with curvature → Second Order (Newton) Methods
  - Can associate sensitivity with some statistics of gradient oscillations, e.g. Adagrad: $M = \mathrm{Diag}\Big(\sqrt{\mathrm{Mean}(g_{1:t}^2)}\Big)$

Mirror Descent

- Mirror Descent (**MD**)
  - General step proximal problem:

    $$\min_x \langle \nabla f(x_0), x - x_0 \rangle + \lambda D(x, x_0)$$

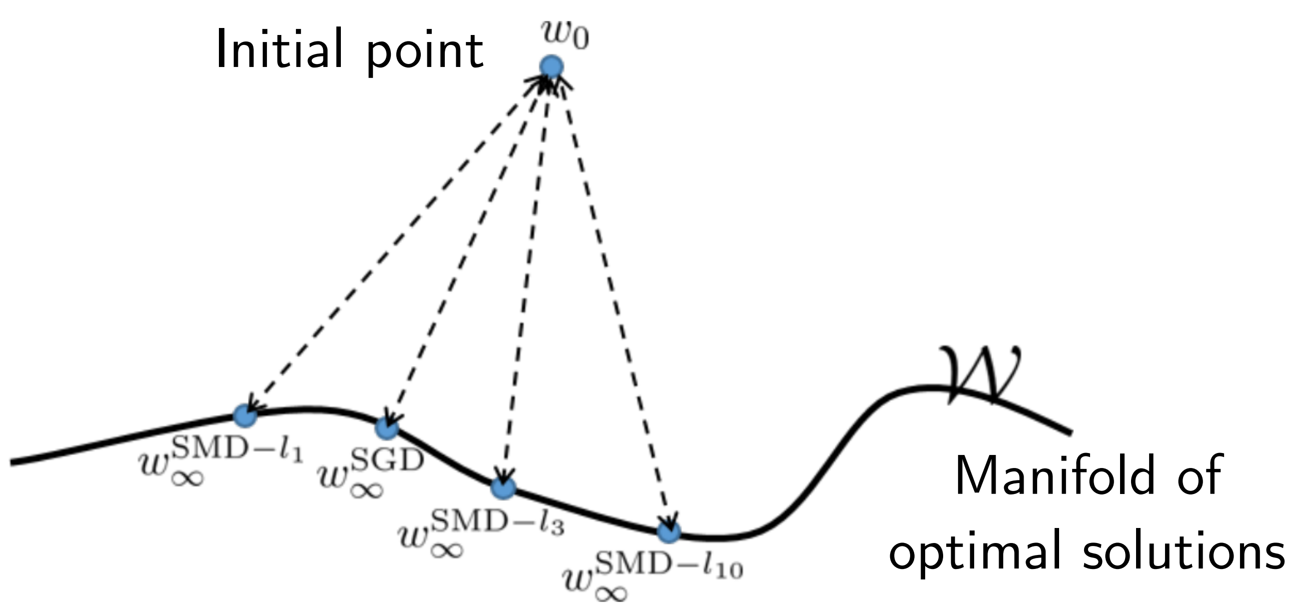
    where D is Bregman divergence (technical details ommitted)
  - We will consider algorithms using unnormalized steps (not solving for λ).
  - Generalizes cases considered so far:

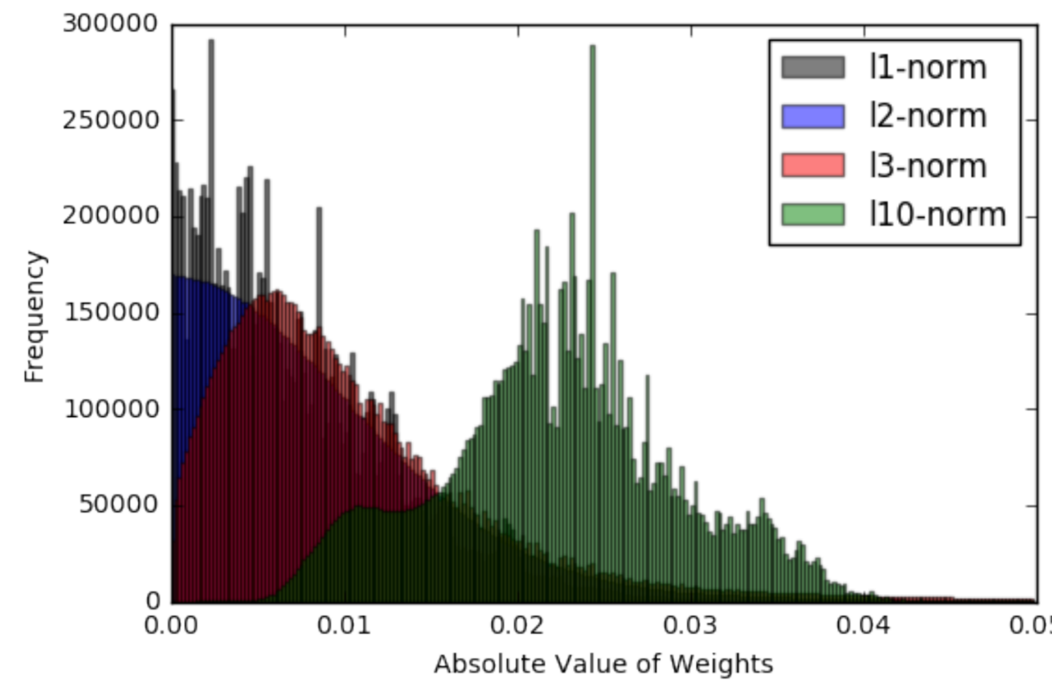
    $D = ||x - x_0||^2$ — (steepest) SGD

    $D = ||x - x_0||^2_M$ — preconditioned SGD

Implicit Regularization by SGD / SMD

- Consider step proximal problem: $\min_x \langle \nabla f(x_0), x - x_0 \rangle + \lambda \|x - x_0\|_p^p$
  - i.e., p-norm stochastic mirror descent
- Using different p leads to solutions with different properties

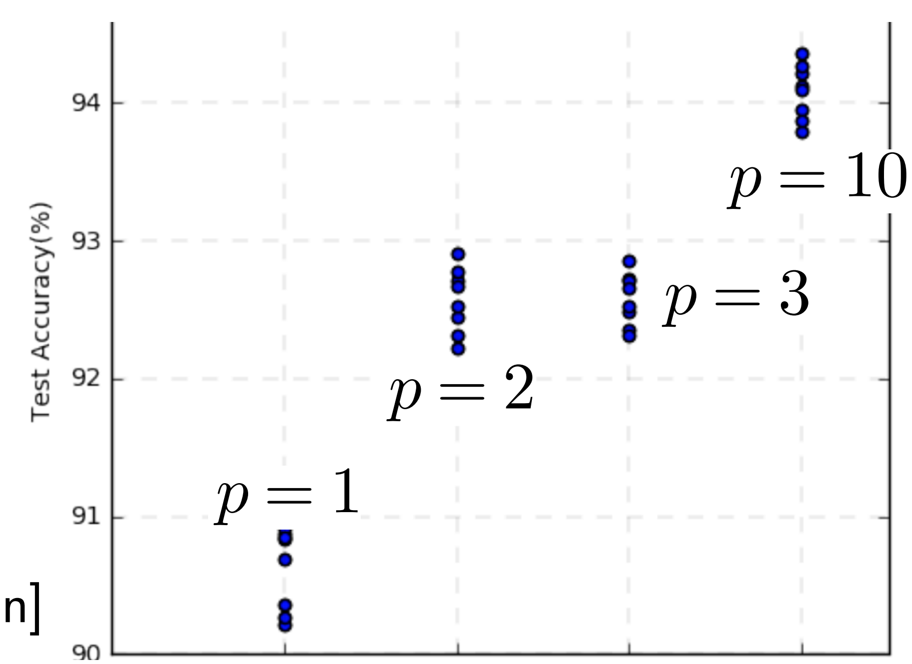




- Iterates tend to $\operatorname{argmin}_{w \in \mathcal{W}} \|w - w_0\|_p^p$, the closest point in the respective norm

	SMD 1-norm	SMD 2-norm (SGD)	SMD 3-norm	SMD 10-norm
1-norm BD	141	9.19×10^3	4.1×10^4	2.34×10^5
2-norm BD	3.15×10^3	562	1.24×10^3	6.89×10^3
3-norm BD	4.31×10^4	107	53.5	1.85×10^2
10-norm BD	6.83×10^{13}	972	7.91×10^{-5}	2.72×10^{-8}

- Different sparsity and generalization

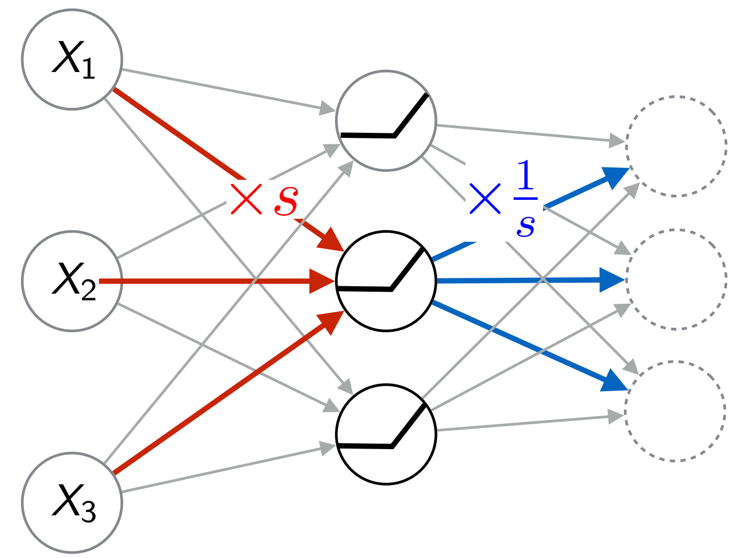


[Azizan et al. (2019) Stochastic Mirror Descent on Overparameterized Nonlinear Models: Convergence, Implicit Regularization, and Generalization]

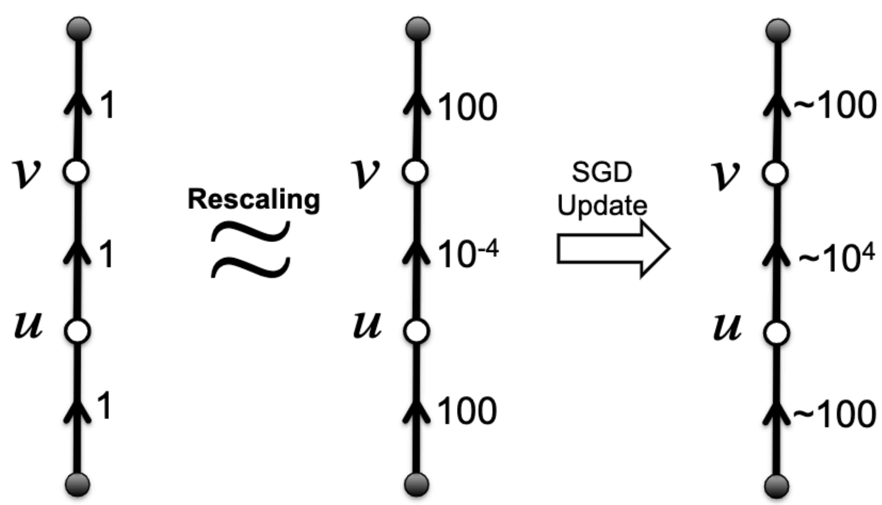
Path-SGD

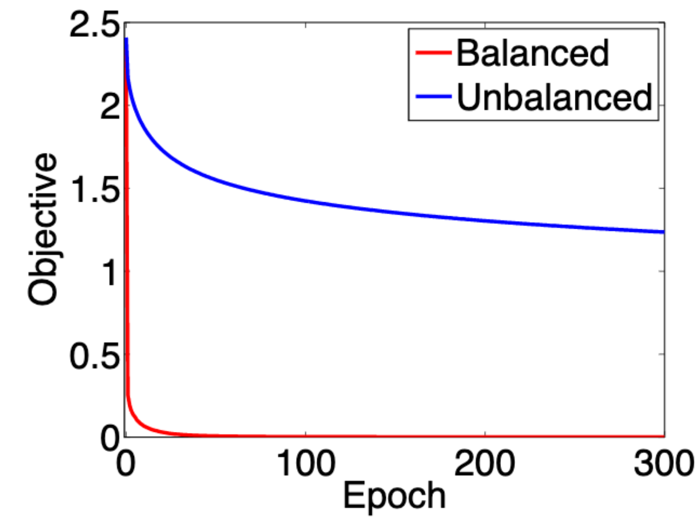
- In ReLU networks we can rescale the weights without affecting the output:
  - ReLU units are *1-homogenous*:
    for $s > 0$: $\text{ReLU}(sx) = \max(0, sx) = s\max(0, x)$
  - Can rescale inputs and outputs of each unit (channels in conv networks)

$$f(Ay) = f(y), \text{ but } J_f(Ay) \neq J_f(y)$$



- Can lead to completely different SGD behavior





(a) Training on MNIST

- Path-SGD considers metric invariant to equivalent transformations.

Prox. problem:
$$\arg\min_{w} \; \eta\left\langle \nabla L(w^{(t)}), w\right\rangle + \left(\sum_{v_{in}[i] \xrightarrow{e_1} v_1 \xrightarrow{e_2} v_2 \dots \xrightarrow{e_d} v_{out}[j]} \left(\prod_{k=1}^{d} w_{e_k} - \prod_{k=1}^{d} w_{e_k}^{(t)} \right)^p \right)^{2/p}$$

[Neyshabur et al. (2015) **Path-SGD**: Path-Normalized Optimization in Deep Neural Networks]

Constrained Optimization with Mirror Descent

✦ Let us use a proximal problem with an appropriate trust region

◆ Mirror Descent (**MD**)

- Use step proximal problem: $\min_x \langle \nabla f(x_0), x - x_0 \rangle + \lambda D(x, x_0)$

  with a suitable divergence D

  (recall previous choices $D = ||x - x_0||^2$, $D = ||x - x_0||_M^2$)
- Very elegant solutions in simple cases

◆ Example: constrained parameter $x > 0$

$D(x, x_0) = x \log \frac{x}{x_0} - x + x_0$ (Generalized KL divergence)

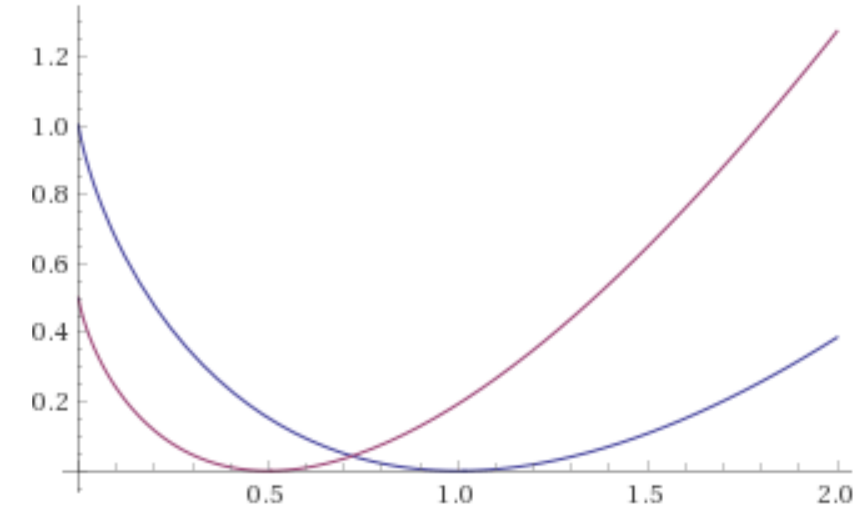
Update: $\log x_{t+1} = \log x_t - \frac{1}{\lambda} \nabla_x f(x_t)$

Note: gradient in x is added to $\log x$

Can implement as:

$y_{t+1} = y_t - \frac{1}{\lambda} \nabla_x f(x_t)$

$x_{t+1} = e^{y_{t+1}}$



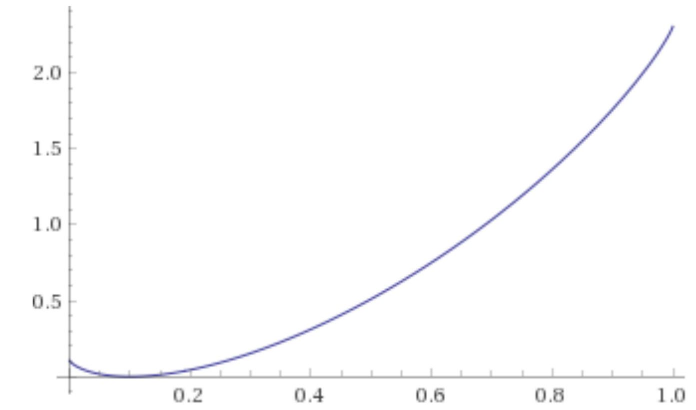
Constrained Optimization with Mirror Descent

- Let us use a proximal problem with an appropriate trust region
- Mirror Descent (**MD**)
  - Use step proximal problem: $\min_x \langle \nabla f(x_0), x - x_0 \rangle + \lambda D(x, x_0)$
    with a suitable divergence D
    (recall previous choices $D = ||x - x_0||^2$, $D = ||x - x_0||_M^2$)
  - Very elegant solutions in simple cases
- Constraint $x \in (0, 1)$

  $D(x, x_0) = x \log \frac{x}{x_0} + (1 - x) \log \frac{1-x}{1-x_0}$ (KL divergence)

  $y_{t+1} = y_t - \frac{1}{\lambda} \nabla_x f(x_t)$

  $x_{t+1} = \mathcal{S}(y_{t+1}) = \frac{1}{1+e^{-y_{t+1}}}$



Constrained Optimization with Mirror Descent

- Constraint $x_i \geq 0$, $\sum_i x_i = 1$ – simplex

  $D(x, x^0) = \sum_i x_i \log \frac{x_i}{x_i^0}$ (KL divergence)

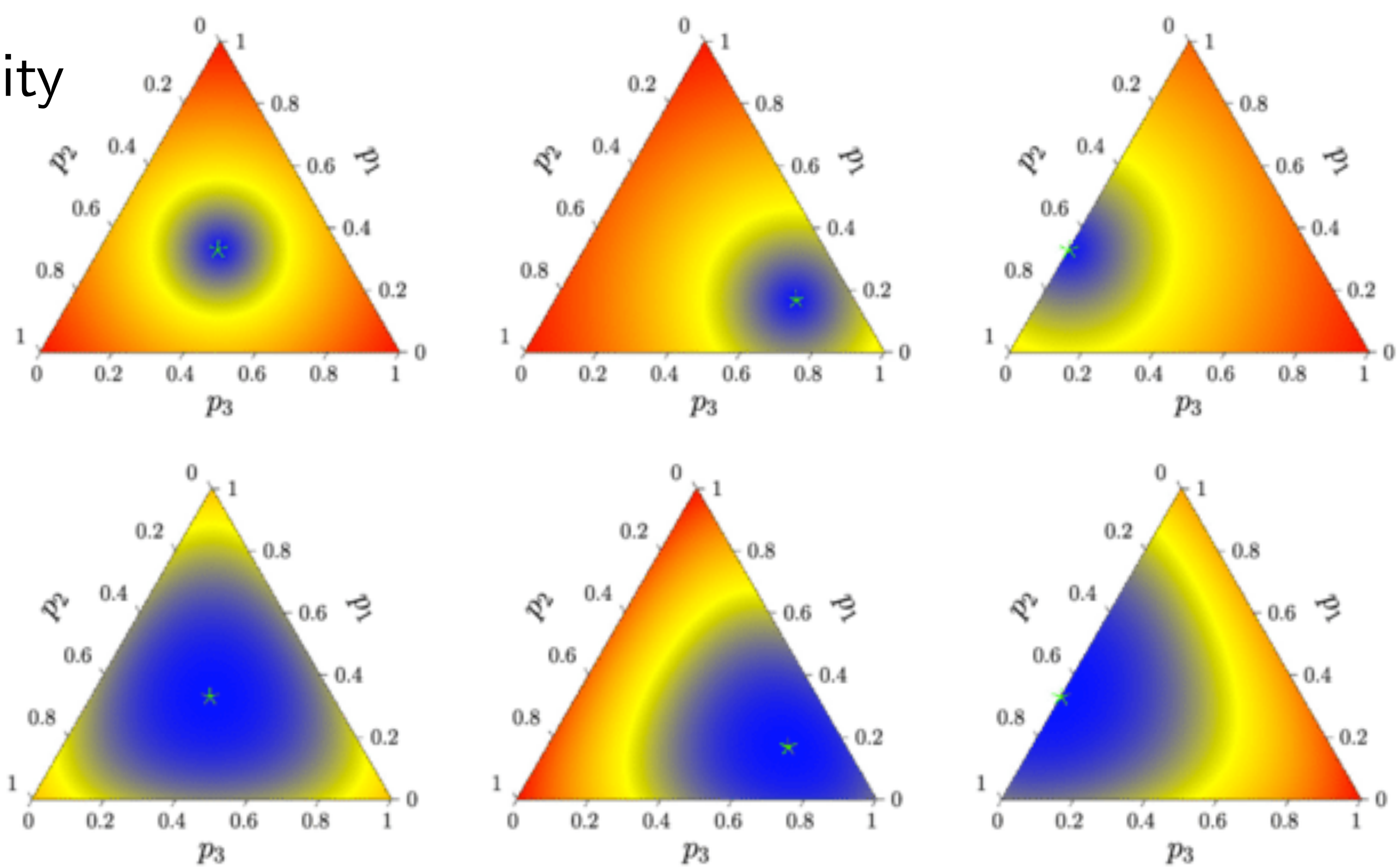
  $y_{t+1} = y_t - \frac{1}{\lambda} \nabla_x f(x_t)$

  $x_{t+1} = \mathrm{softmax}(y_t + 1)$

  - Can substitute and get update of x directly → **exponentiated GD** ($\star$)

Quadratic fidelity

KL fidelity



- Convergence in stochastic non-convex setting?
- At least we clearly see it averages gradients in the "mirror" space. Works in practice.

Why not Simpler ways to Handle Constraints?

- **Example**: Need a parameter that models variance σ^2 of some distribution inside NN
  - Must be $\sigma^2 > 0$
  - But do not know the scale, e.g. $\sigma^2 \in [10^{-4}, 10^4]$

  Option 1: projected GD

  Parametrize as $\sigma^2 = y$

  Projecting to $y \geq 0$ may result in invalid variance

  Cannot recover small σ^2 more accurately than the step size

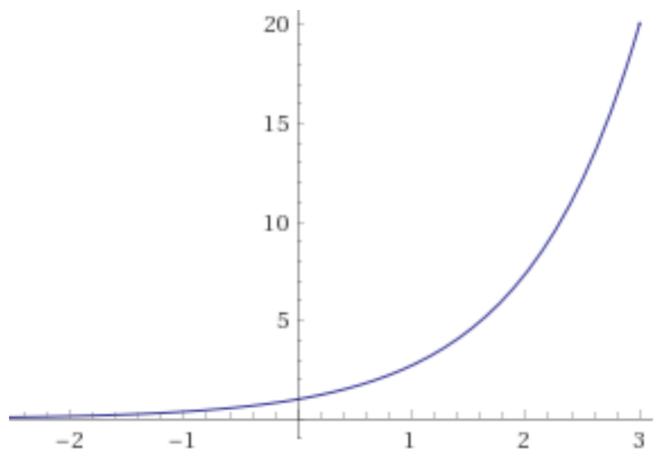
  May never make enough steps to find big σ^2

  Option 2: Parametrize as $\sigma^2 = e^y$, $y \in \mathbb{R}$

  May overflow for large y

  Gradients grow unbounded

  If stepped to small values of y accidentally, gradients vanish

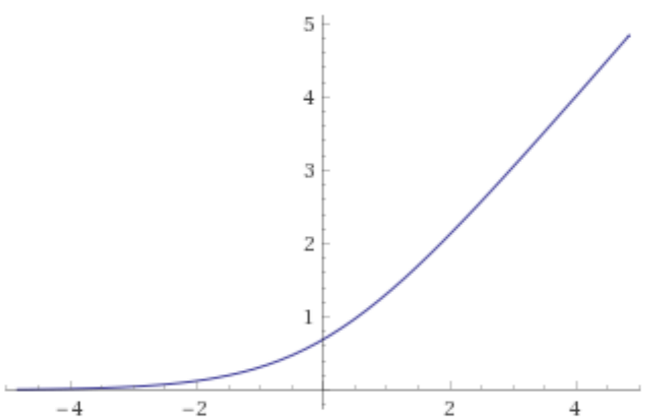


  Option 3: Parametrize as $\sigma^2 = \log(1 + e^y)$, $y \in \mathbb{R}$

  Gradients bounded

  May vanish if we step to $y \ll 0$

  May never get to high range values



(All options work to some extend, in particular Option 3 is often used in literature)