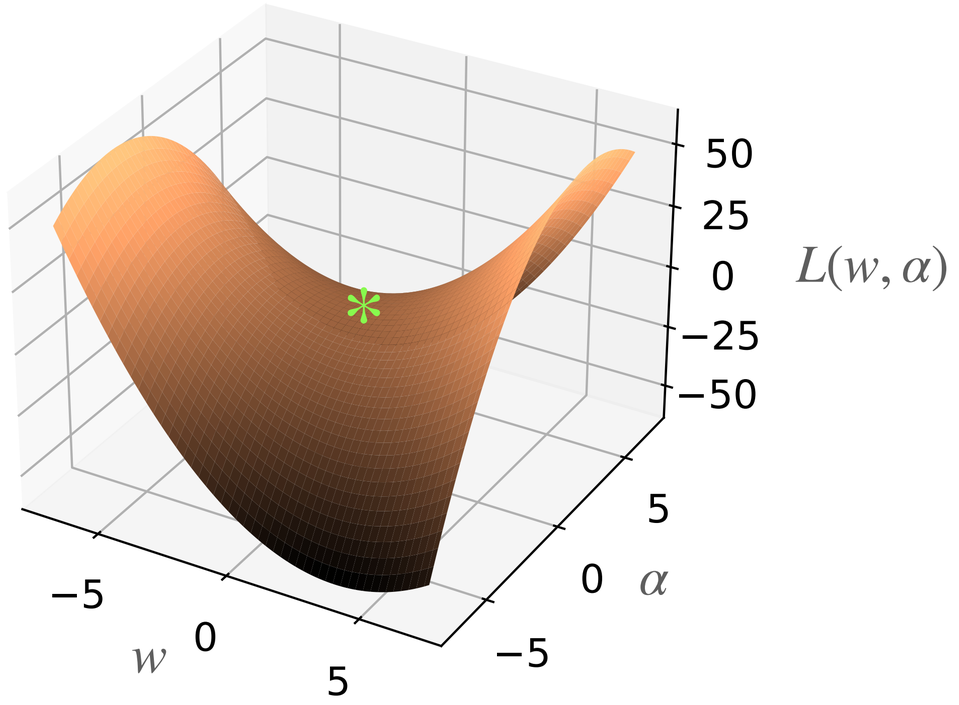
Duality

10-701 Introduction to Machine Learning

Geoff Gordon and Pradeep Ravikumar

Adversarial (min-max) problems



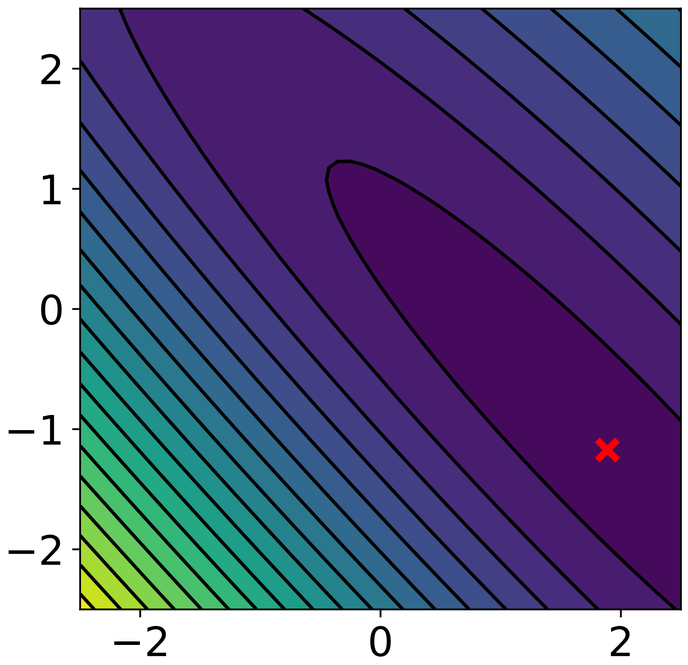
- So far we've looked at problems of form $\min_w L(w)$
- Some ML problems instead have form $\min_w \max_\alpha L(w, \alpha)$
  - often called *adversarial learning:* the w player and α player have opposing goals
  - a (local) optimum is a point where w can't (locally) decrease and α can't (locally) increase objective value
  - (locally) convex-concave, looks like a saddle: *saddle-point*

Algorithms

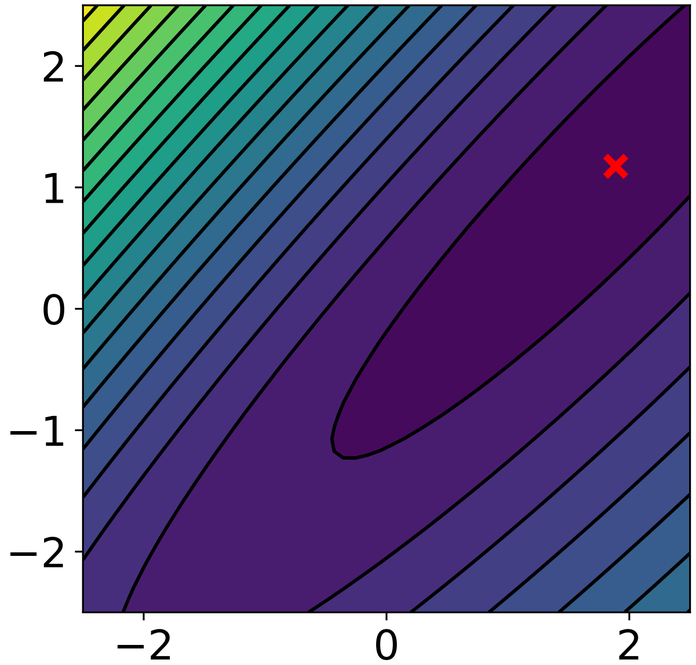
- Idea: ***(stochastic) gradient descent-ascent (S)GDA***
  - min player runs (stochastic) gradient descent (maybe with momentum, Adam, etc.)
  - max player runs (stochastic) gradient ascent, interleaved
  - kind of works, no guarantees — people force it w/ hyperparameter tuning (learning rate schedules, update frequencies, …)
- There exist methods with better guarantees: ***no-regret*** learning, ***optimistic*** (S)GDA
  - they seem not to be used that much in practice
  - hypothesis: they hurt the mystical properties of SGD while helping convergence
  - and some guarantees don’t extend to practical situations
  - and some methods require inconvenient modifications like storing extra copies of our network

Example: problem splitting

Learner 1 loss function



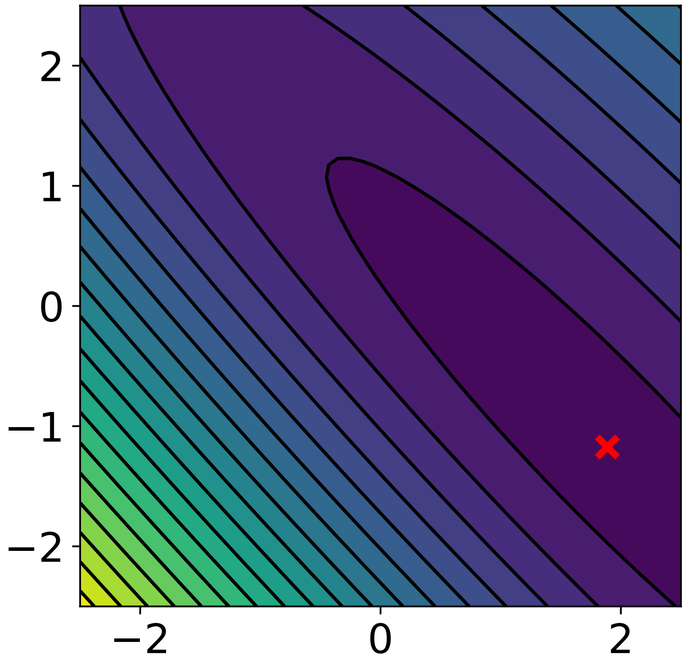
Learner 2 loss function



- Two learners, each with half of our dataset
  - for speed with big dataset
  - or for privacy: e.g., two hospitals unwilling to share full patient records

Example: splitting data

Learner 1 loss function



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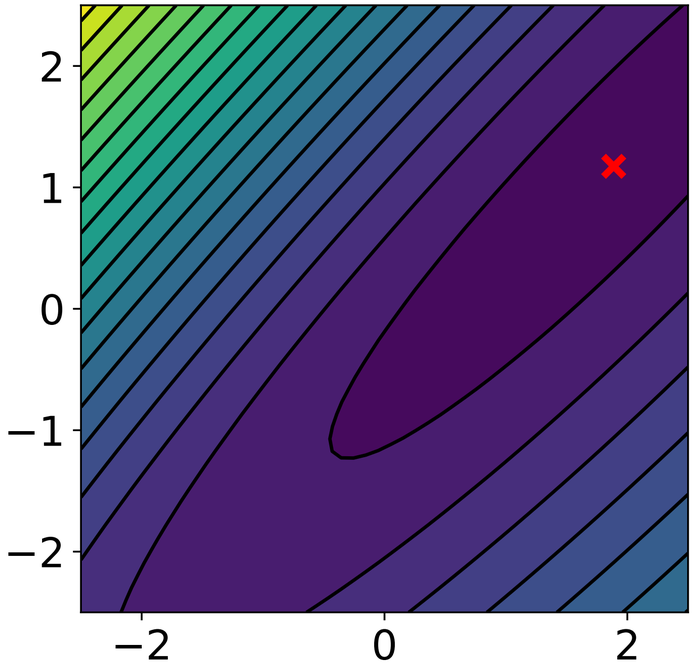

- If optimized independently: $\min_{\theta_1} L_1(\theta_1)$, $\min_{\theta_2} L_2(\theta_2)$
- Best solution: $\min_{\theta_1,\theta_2} \left[L_1(\theta_1) + L_2(\theta_2)\right]$ s.t. $\theta_1 = \theta_2$
  - equivalent to centralized answer $\min_{\theta} \left[L_1(\theta) + L_2(\theta)\right]$

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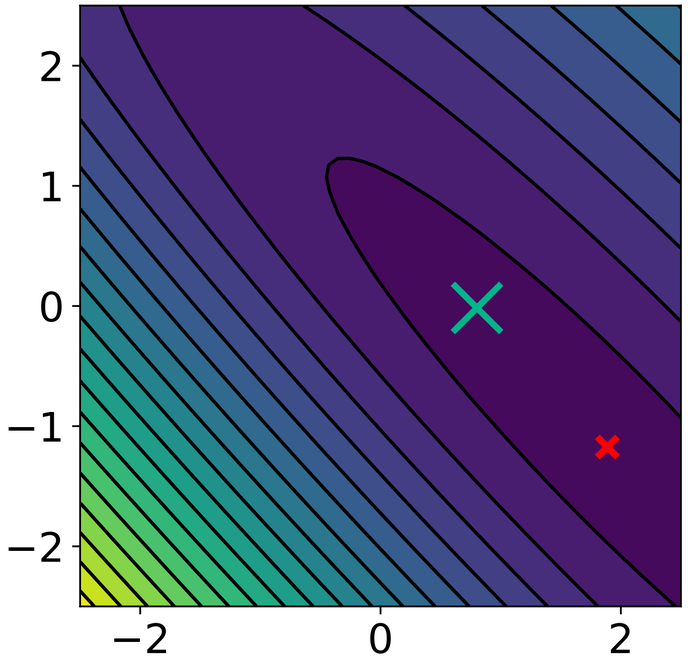

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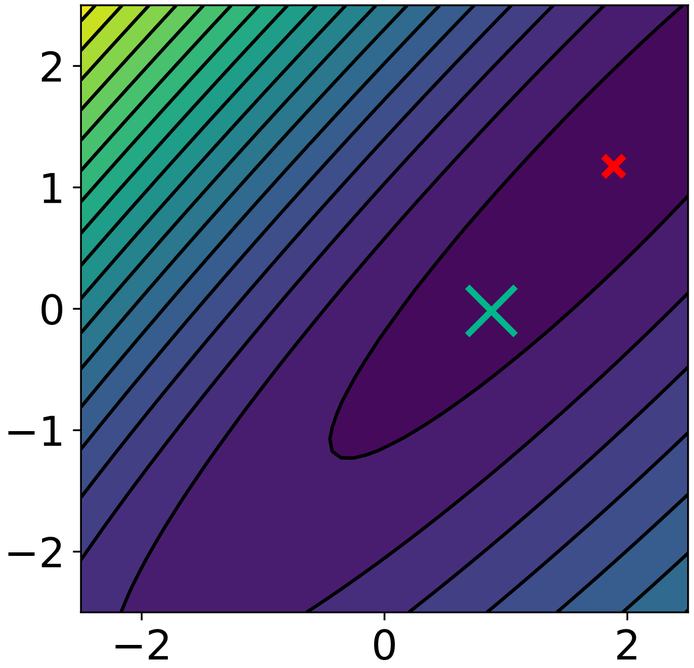

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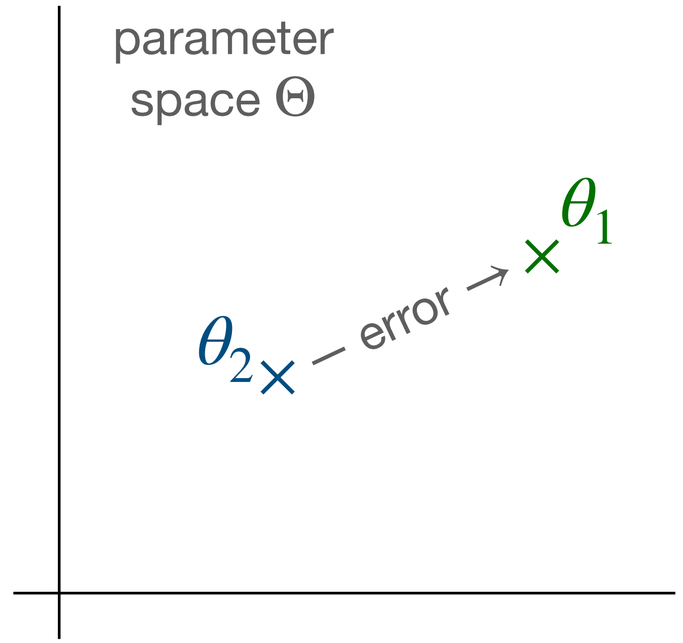
Lagrange multiplier



- To enforce the equality constraint, add an adversary that searches for and penalizes violations
  - $\min_{\theta_1,\theta_2} \max_m \left[L_1(\theta_1) + L_2(\theta_2) + m^\top(\theta_1 - \theta_2)\right]$
- The θ_1, θ_2 players lose badly (loss $+\infty$) if they choose $\theta_1 \neq \theta_2$

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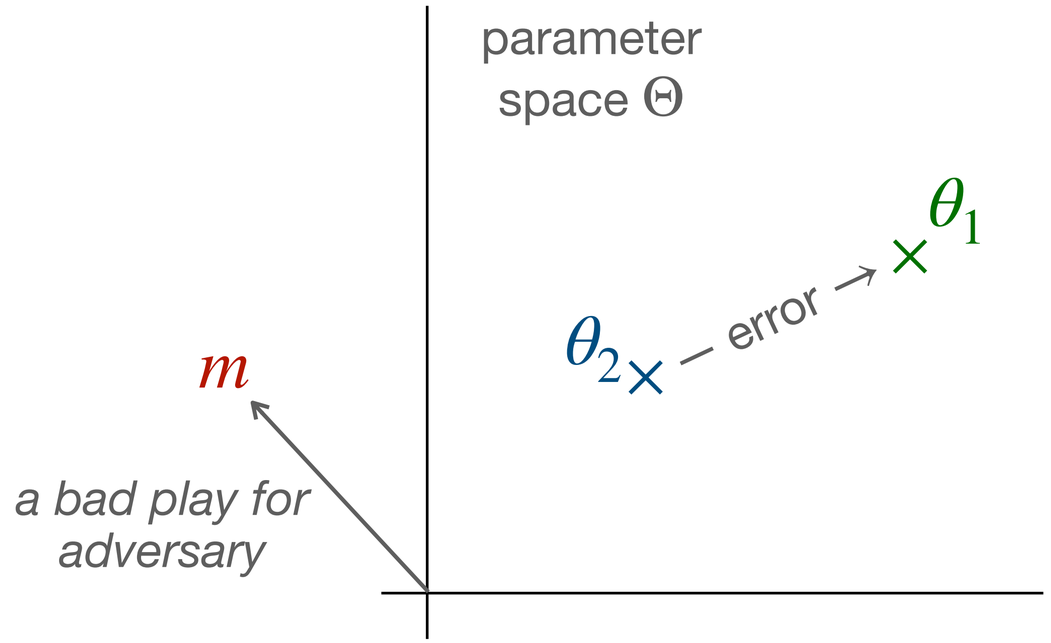

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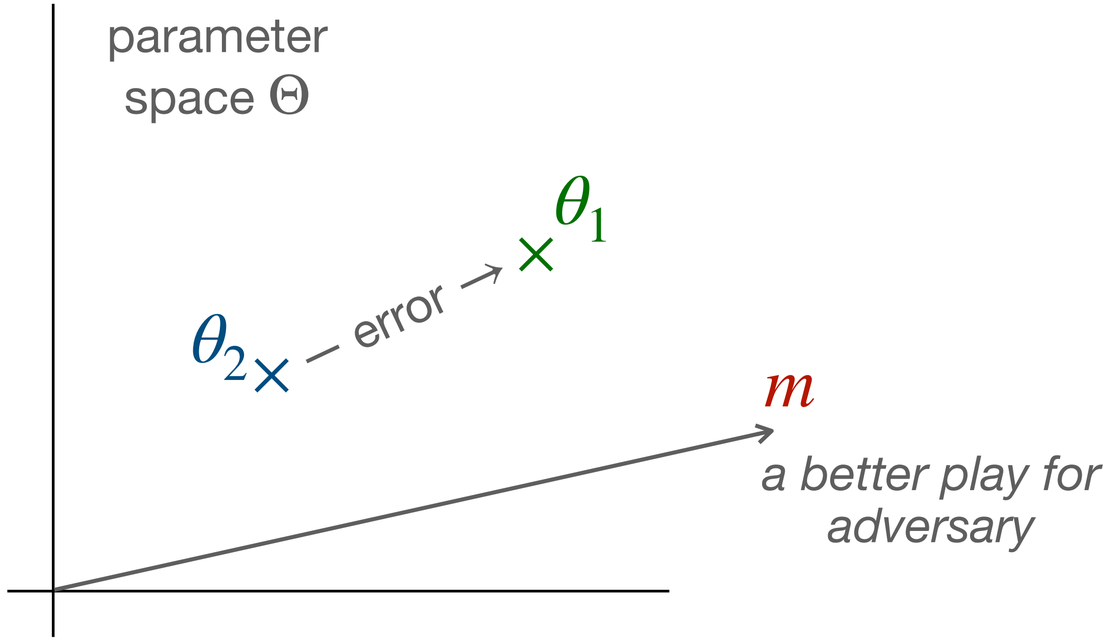

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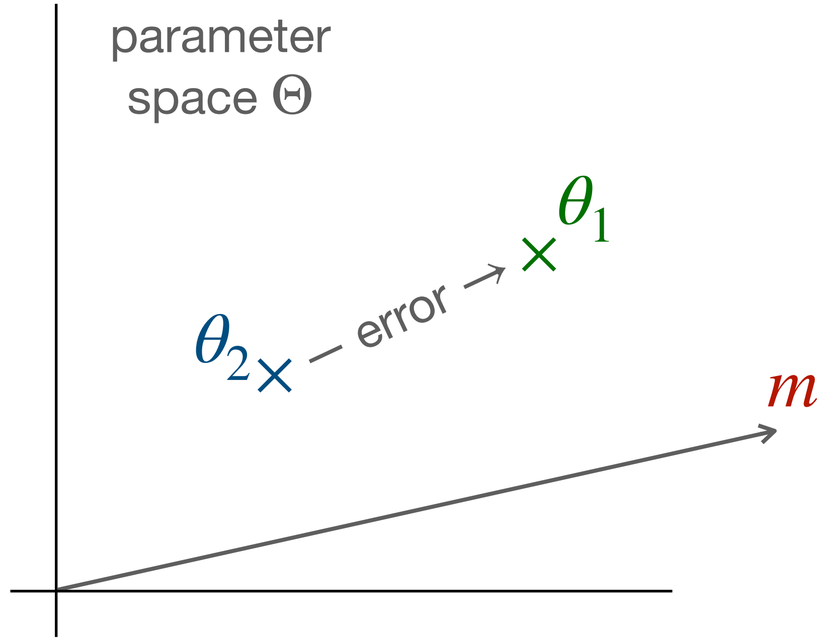
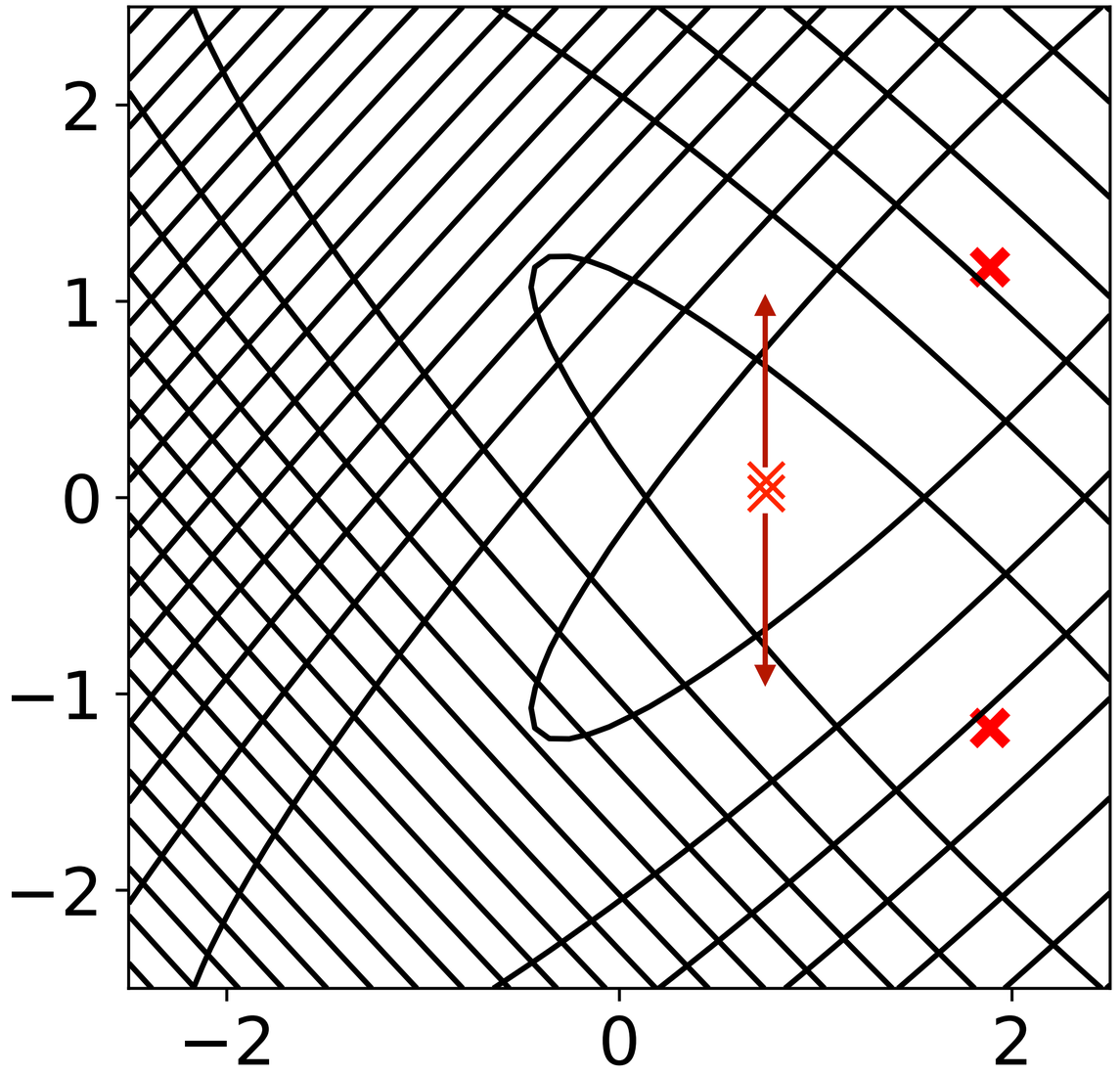
Adversary corrects constraint violations



- Now θ_1 player and θ_2 player can optimize mostly independently — if we fix m the problem splits:
  - $\min_{\theta_1} \left[L_1(\theta_1) + m^\top \theta_1 \right]$ and $\min_{\theta_2} \left[L_2(\theta_2) - m^\top \theta_2 \right]$
- And if we fix θs, good plays for adversary are directions that encourage θ_1 and θ_2 to move closer together

Equilibrium



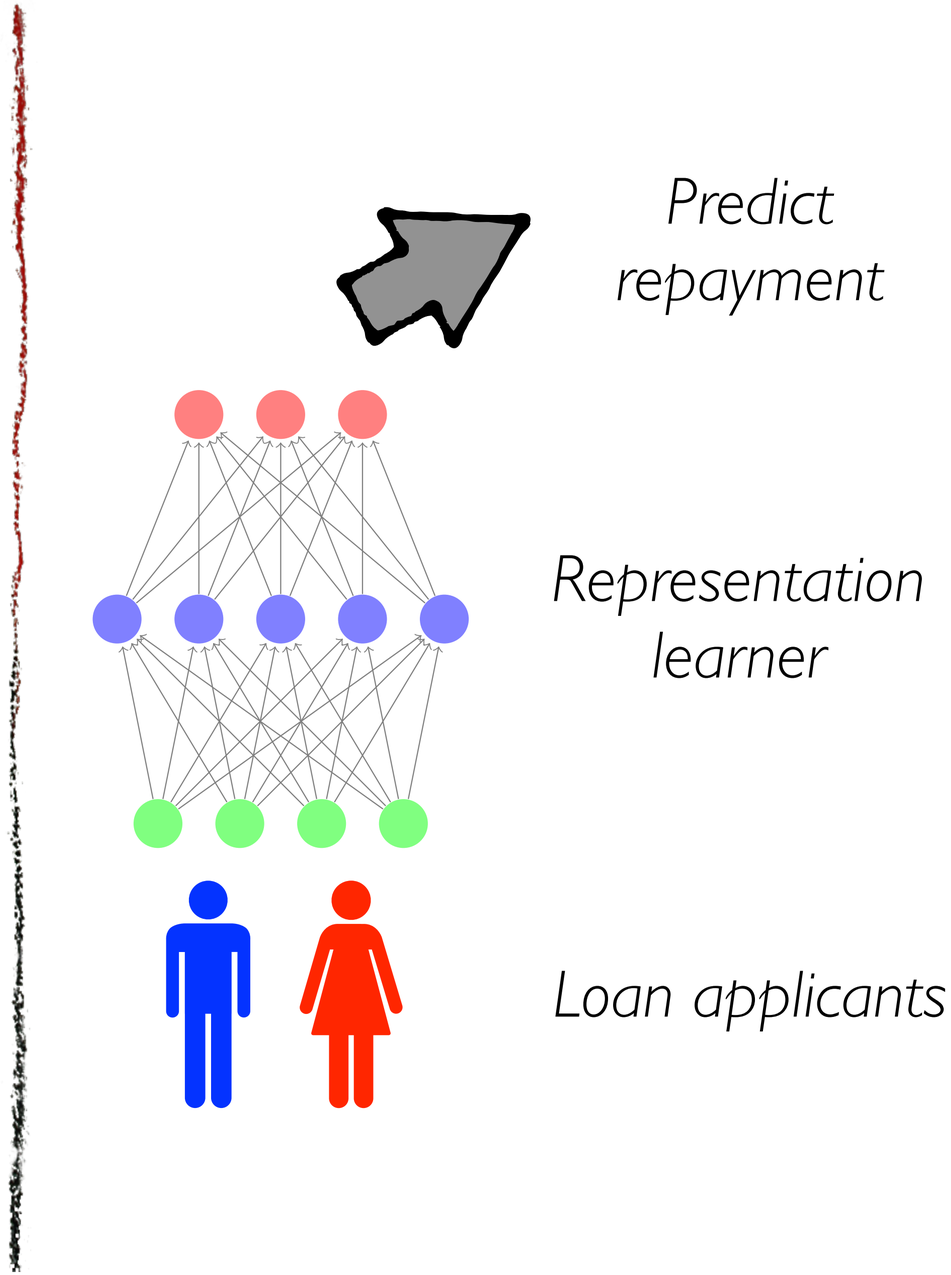
- If everyone learns at once, we hope to converge to a (local or global) optimum, called an ***equilibrium****:* gradient for each player = zero, no incentive to move

Finding the equilibrium

$$\min_{\theta_1,\theta_2} \max_m \left[L_1(\theta_1) + L_2(\theta_2) + m^\top(\theta_1 - \theta_2)\right]$$

- Find equilibrium by setting gradients wrt θ_1, θ_2, m to 0:
  - $0 = \nabla_m =$
  - substitute back in:

Example: fairness

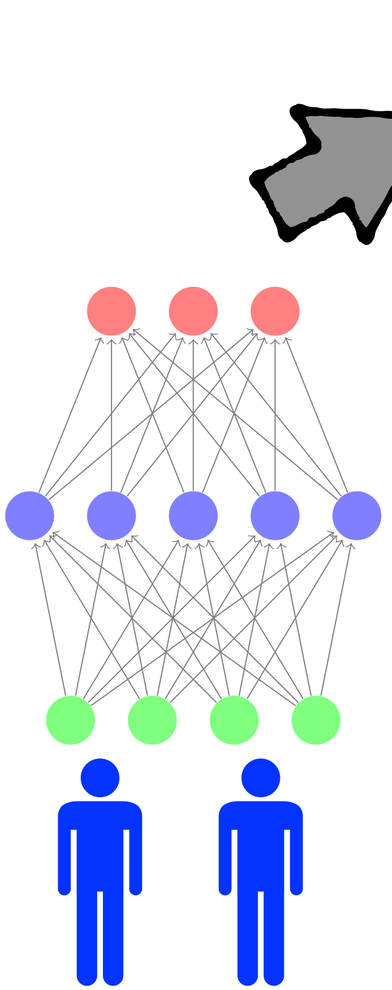


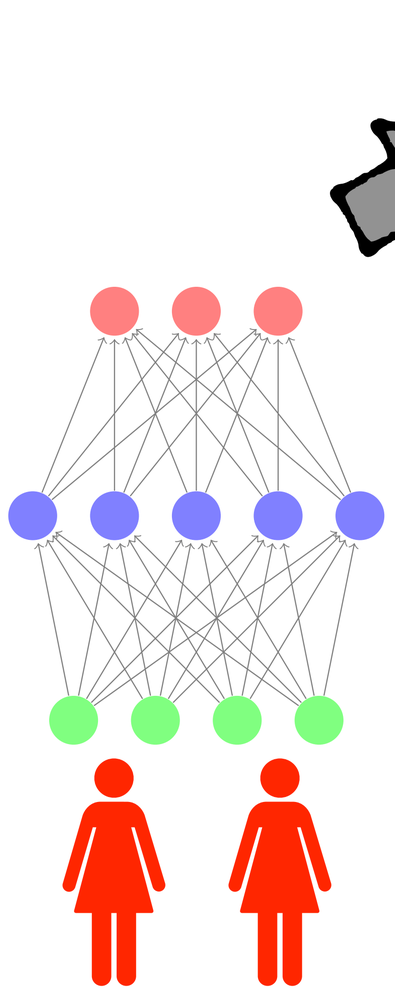
- ***Problem:*** naive classifier can't be better than the dataset we start from!
  - Human loan officers used different criteria to approve women and men
  - Systemic biases made equally qualified candidates more or less likely to repay
- In fact, often worse: ML learns to apply bias more consistently and effectively
- We can do *better at prediction* by doing *worse at minimizing holdout error*

"Apple Card algorithm sparks gender bias allegations," Washington Post, Nov 2019

Enforce constraints to improve fairness

reduce training set accuracy to improve generalization





- Constrain $P(\text{repay} \mid \text{M}) = P(\text{repay} \mid \text{F})$
  - statistical parity (independence)

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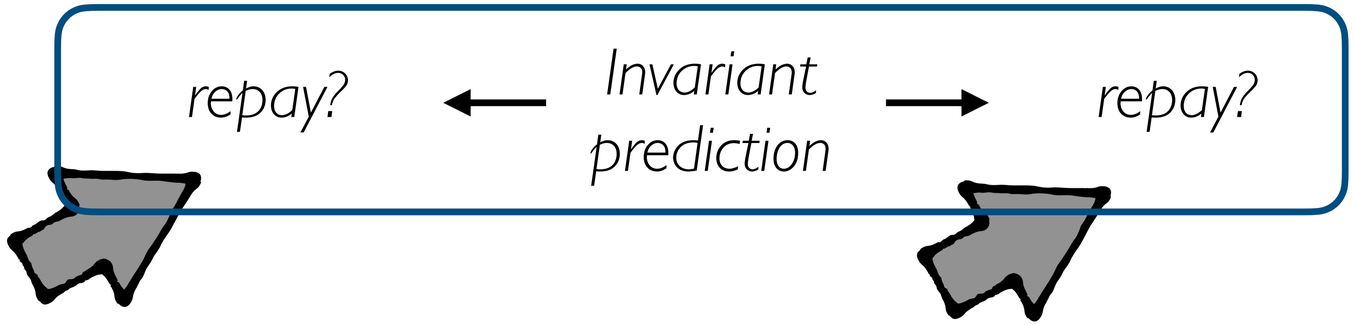

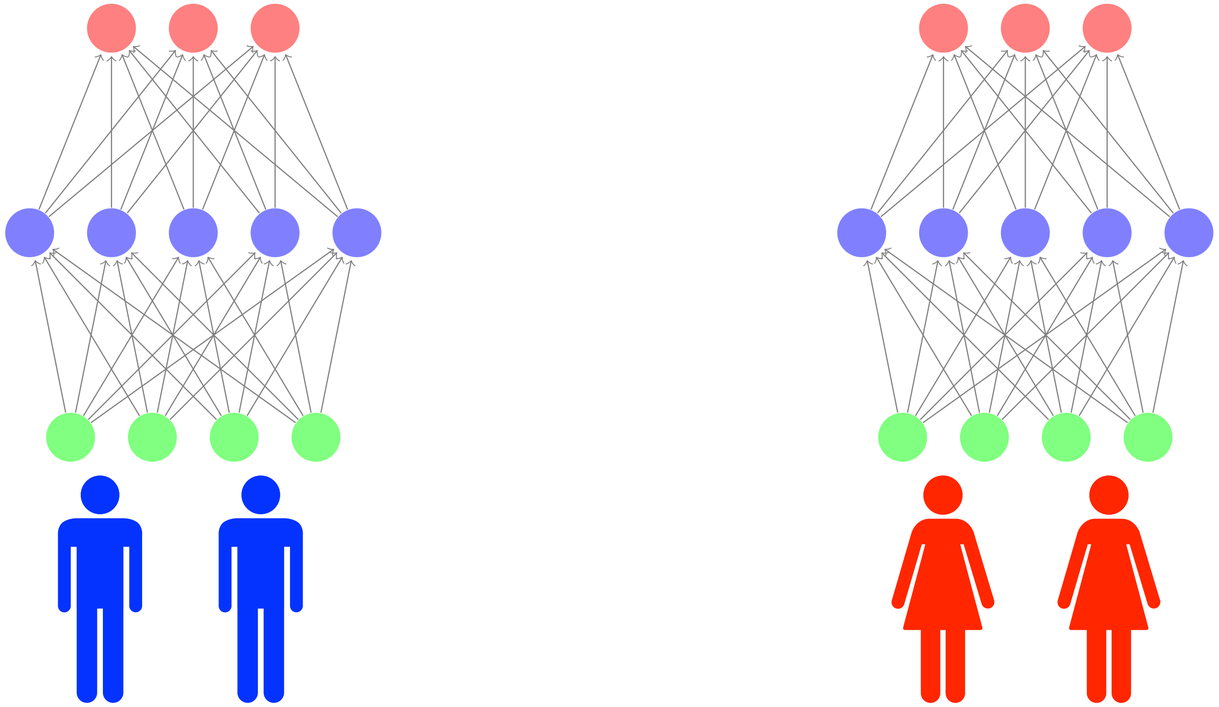

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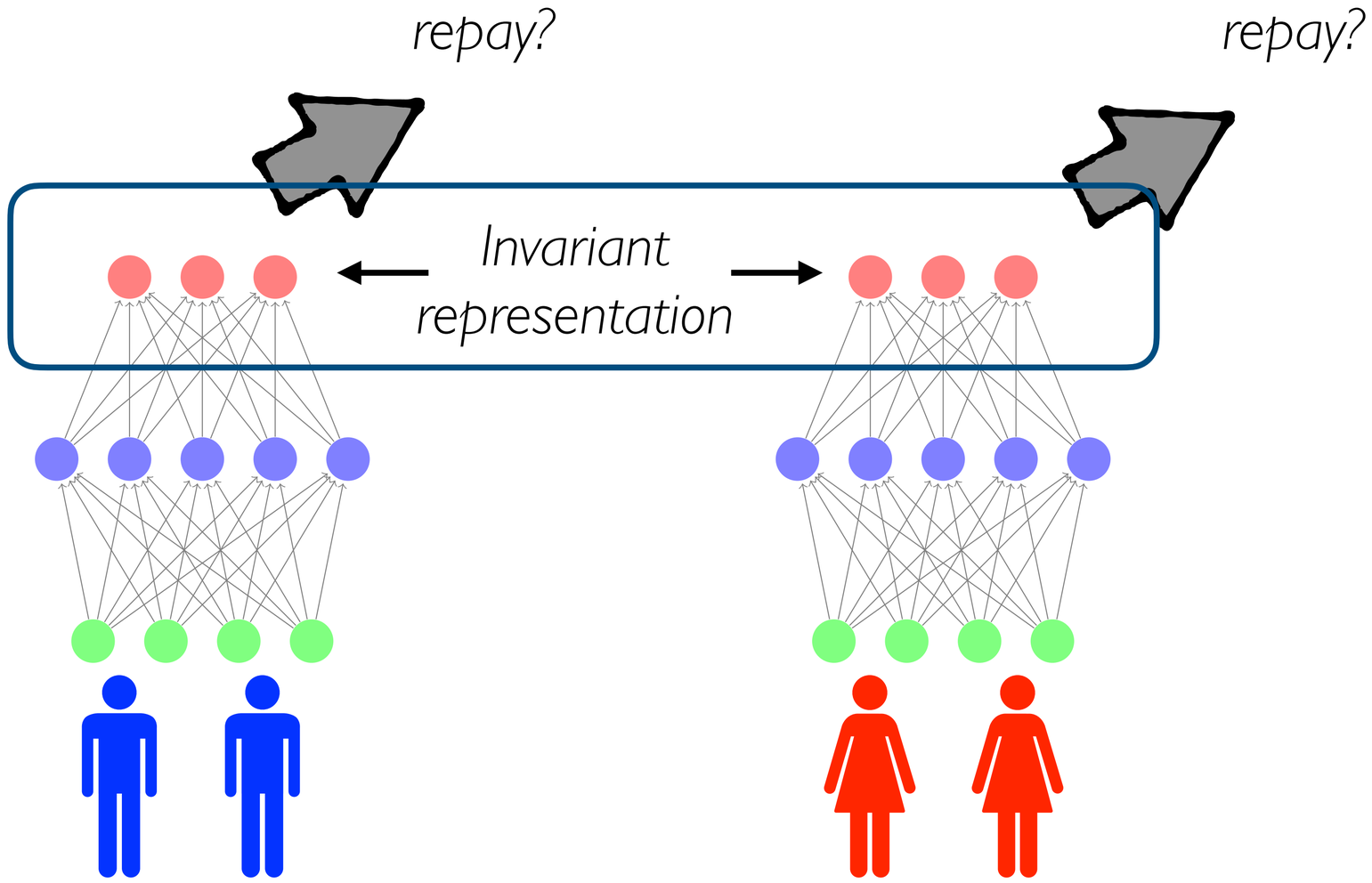
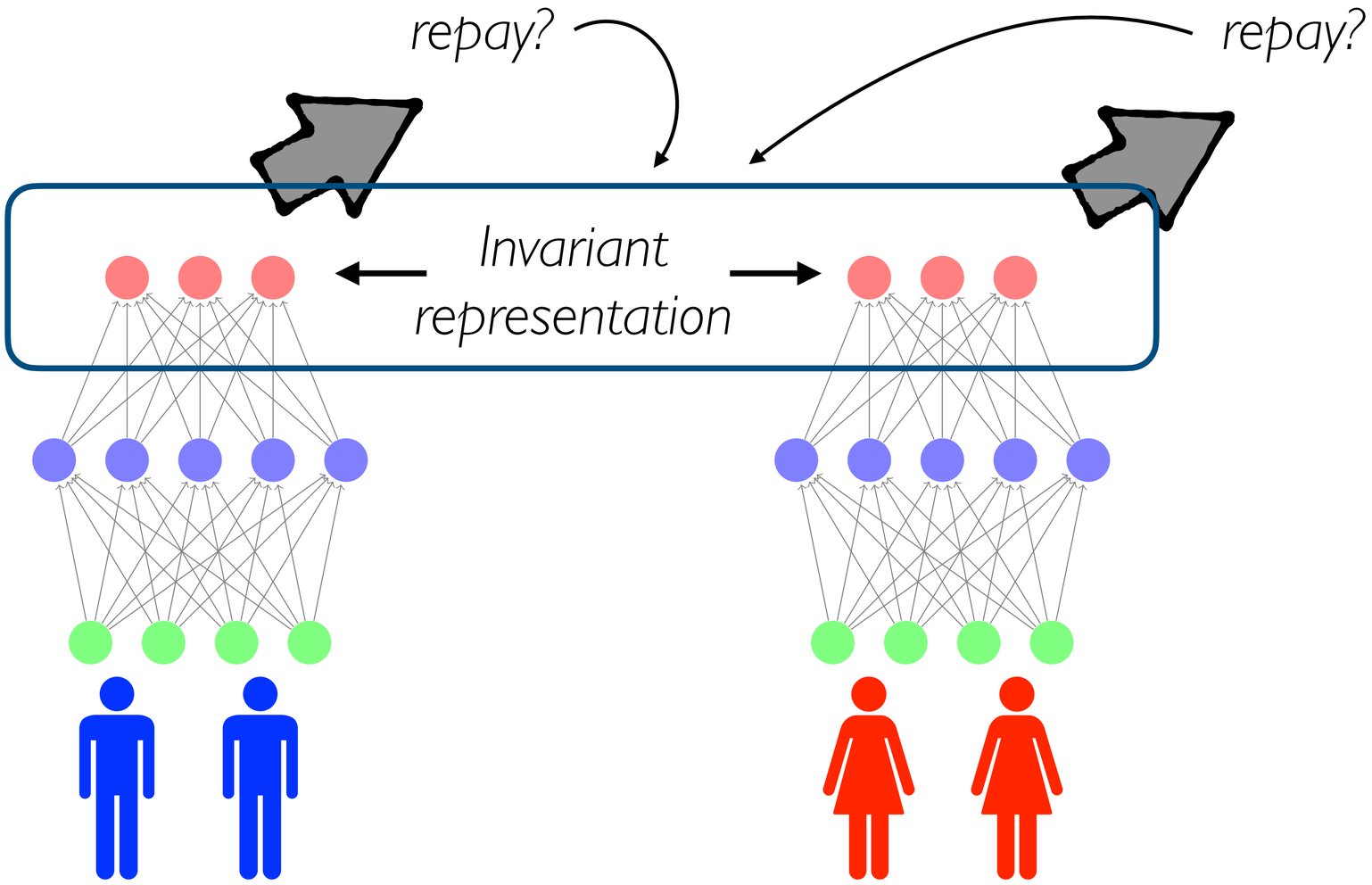


- Constrain $P(\text{representation} \mid \text{M}) = P(\text{representation} \mid \text{F})$
  - statistical parity, but maybe more robust

Enforce constraints to improve fairness

reduce training set accuracy to improve generalization



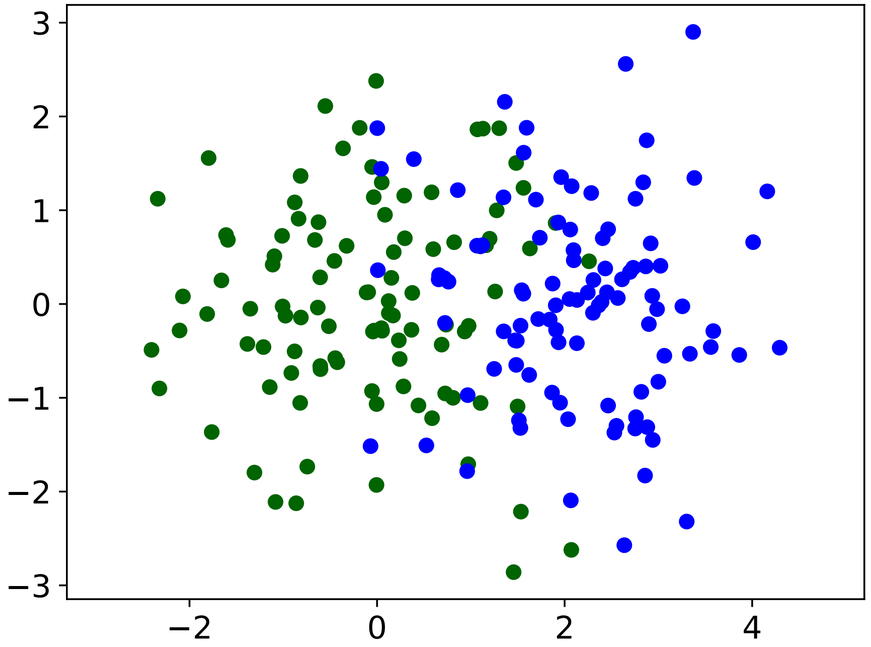
- $P(\text{representation} \mid \text{M}, \text{repay}) = P(\text{representation} \mid \text{F}, \text{repay})$
  - separation: representation (and therefore prediction) $\perp$ M/F given true label

Adversary

- Can express any of these constraints with an adversary
  - independence by invariant prediction: scalar constraint, adversary is a single real Lagrange multiplier
  - independence by invariant representation: much more complicated constraint, adversary needs to be an ML model
    - a ***discriminator*** that tries to classify representations to predict whether they came from M or F
    - if $P(\text{M} \mid \text{representation}) \neq P(\text{F} \mid \text{representation})$, adversary can win (equivalent to constraint above)
  - separation by invariant representation: discriminator now sees both representation and true label, predicts M/F
- Soft constraint: $\min_\theta \max_\phi \underbrace{L(\theta)}_{\textit{original loss}} + \lambda \underbrace{D(\phi)}_{\textit{discriminator}}$

ML model as adversary (discriminator)

- Suppose our two groups have different distribution of representations:



- Optimal discriminator tells us how they differ

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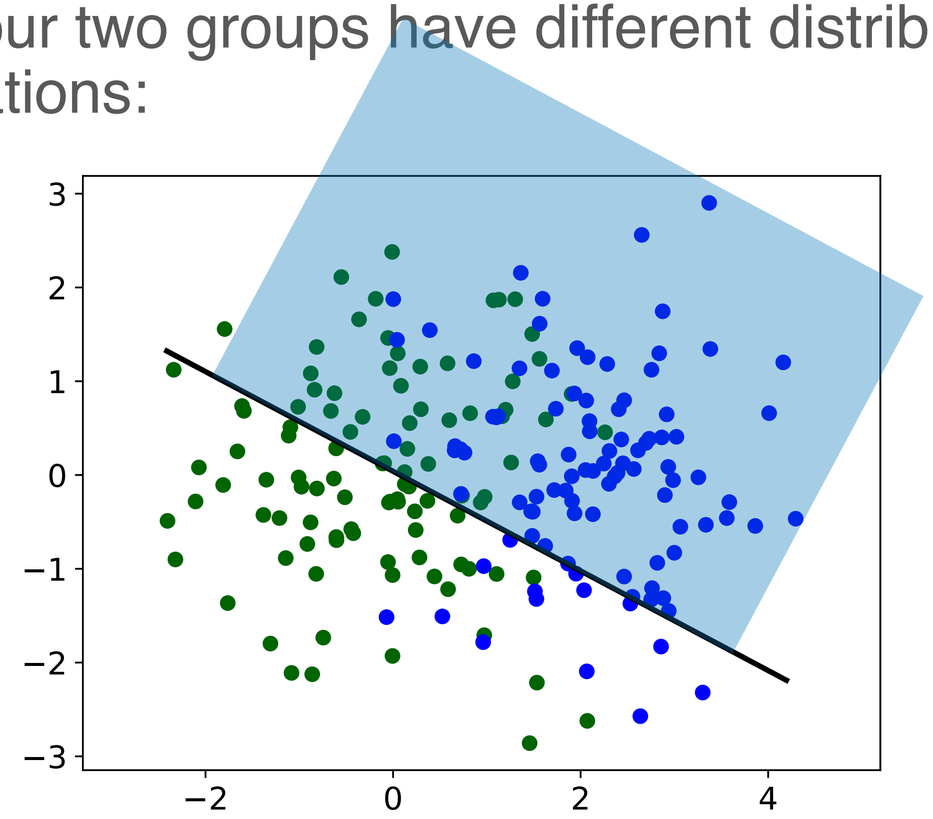

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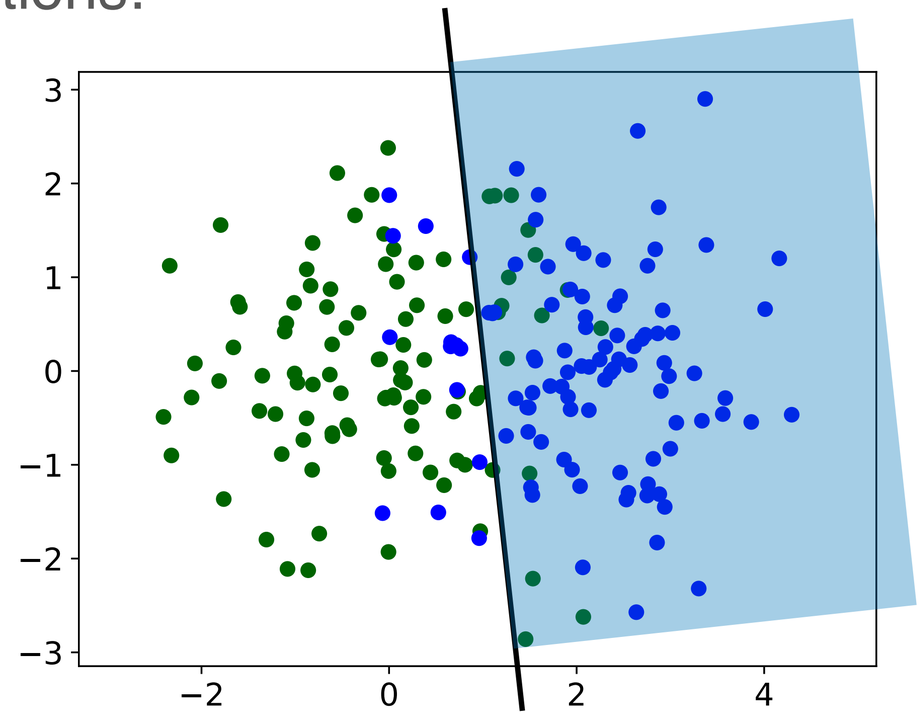

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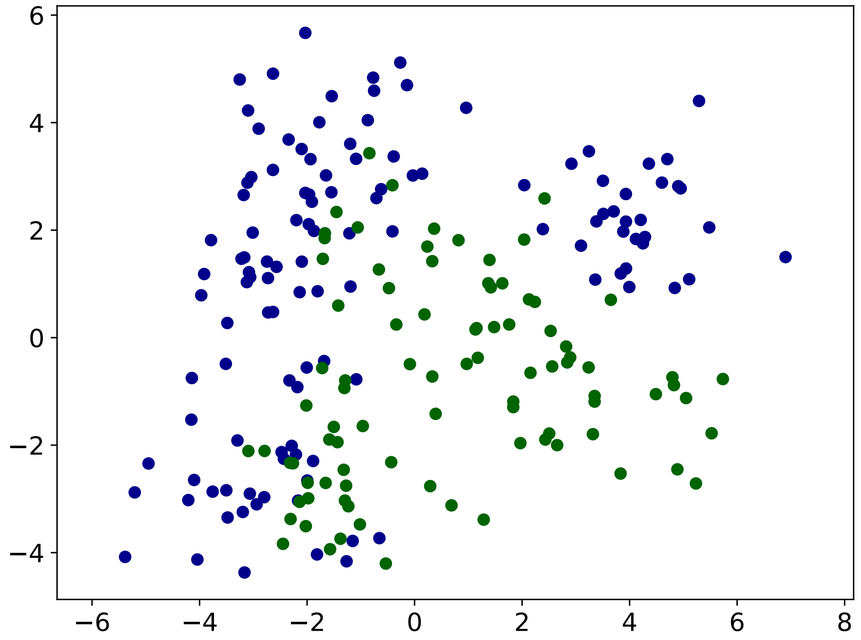

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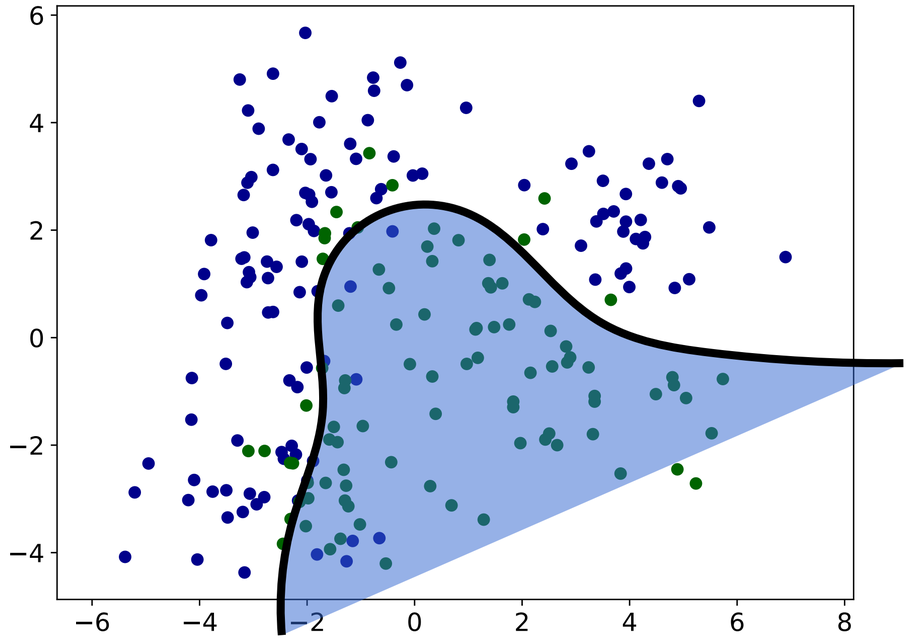
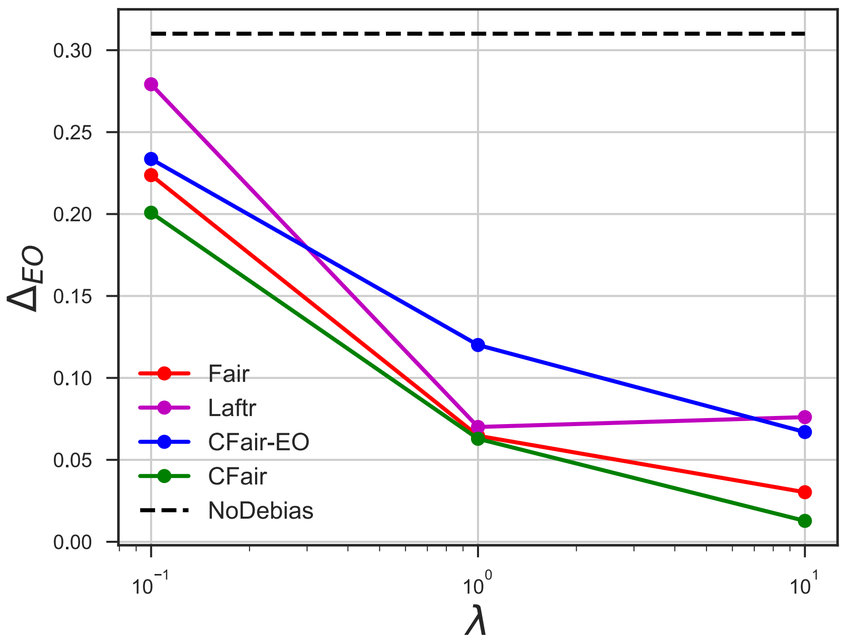
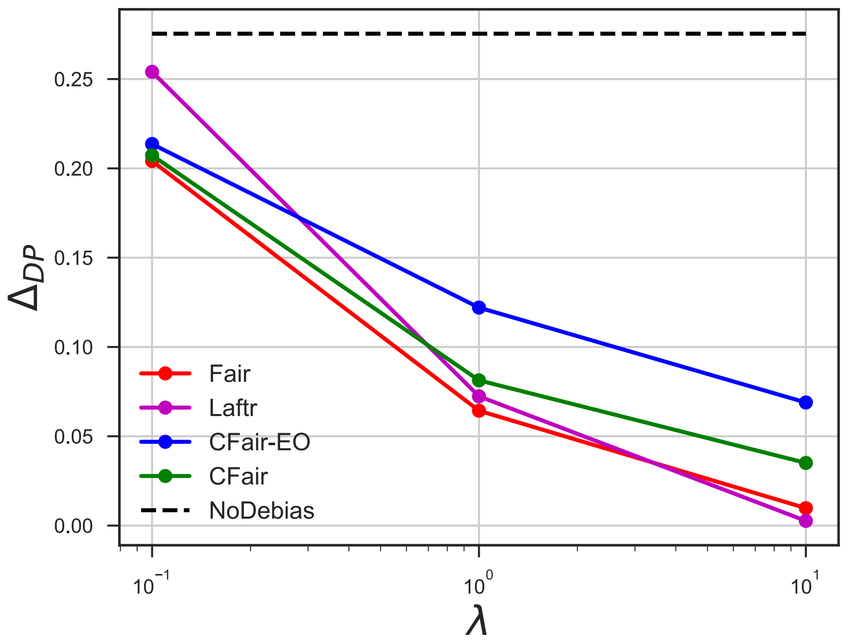


- Optimal discriminator tells us how they differ

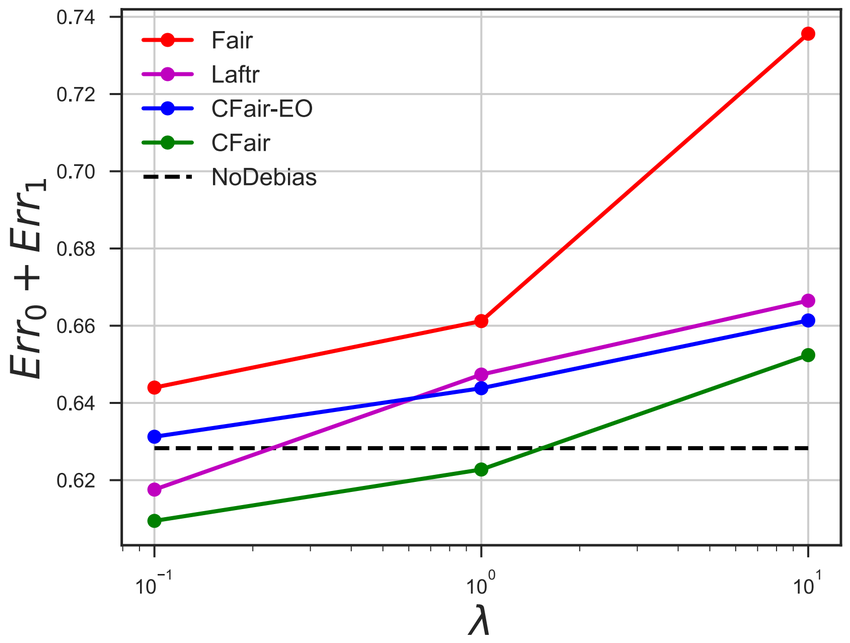
observed separation (equality of odds)



observed independence (demographic parity)



observed error rate



Experiment

- Compare observed separation, independence, and error rate for different soft constraints (strength λ)
  - – – no constraint; —— independence; —— separation
  - constraints enforced on *invariant representation*
- Separation seems to achieve a good tradeoff

[Zhao et al., ICLR 2020]

Example: generative adversarial networks

- Another constraint that's tough to represent:
  - train a neural net (generator) applied to a noise input: $f_\theta(z)$
  - goal: output distribution should match some given samples (e.g., cat pics downloaded from internet)
  - variant: *conditional* generation: generate cat pics on input "cat", ferret pics on input "ferret"
- Approach:
  - add an adversary (discriminator): classifier with parameters ϕ, maps images to real-valued score
  - discriminator tries to adjust ϕ to recognize generated images vs. real sampled cat pics: +ve score for real, –ve for generated
  - generator tries to adjust θ to fool discriminator

GAN min-max objective

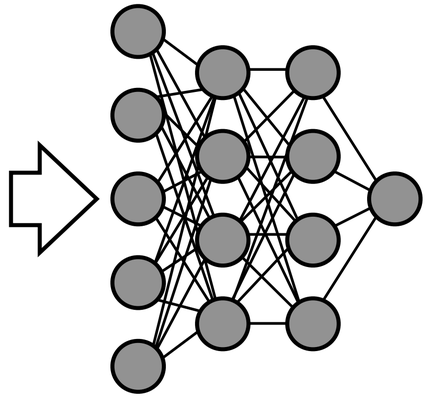
overall log likelihood:

$$\frac{1}{2}\mathbb{E}(\ln P_\phi(-1 \mid f_\theta(z^{(i)}))) + \frac{1}{2}\mathbb{E}(\ln P_\phi(+1 \mid x^{(i)}))$$

noise samples $z^{(i)}$, real samples $x^{(i)}$

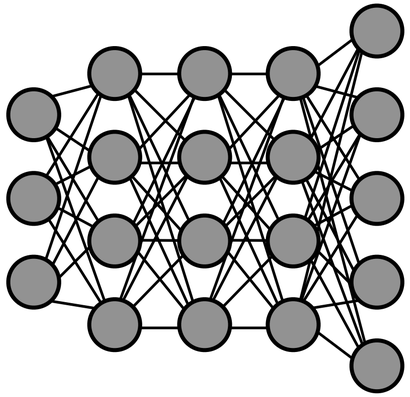
(many variations proposed)

real image

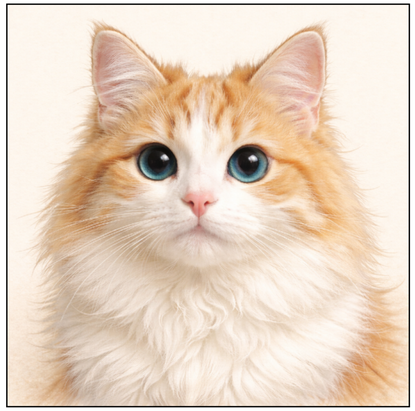


discriminator P_ϕ

noise



generator f_θ



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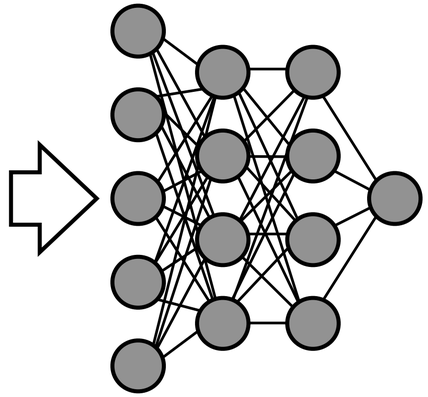

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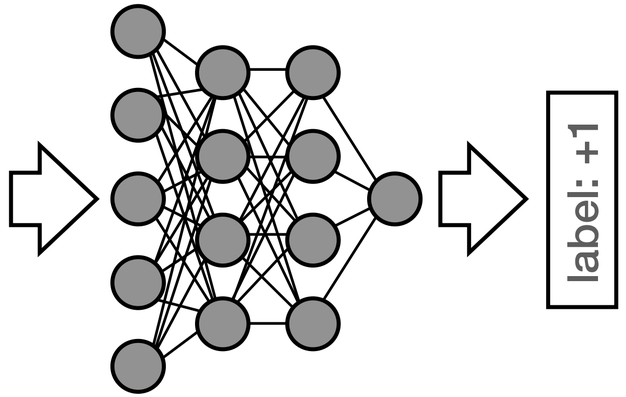
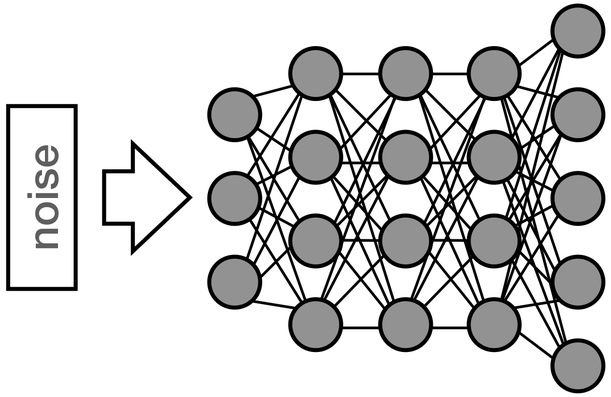


discriminator P_ϕ

min log likelihood wrt θ



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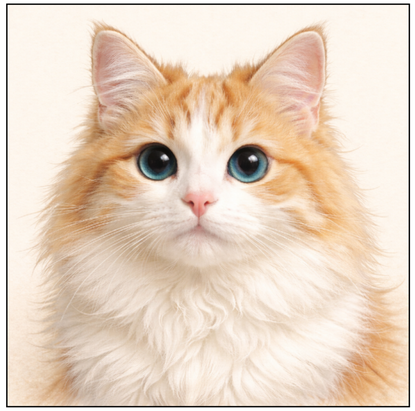

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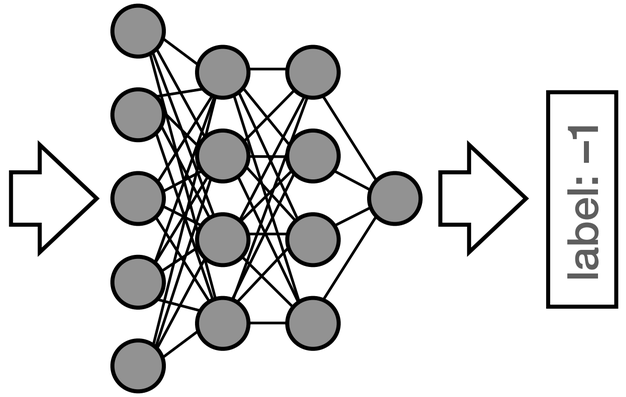

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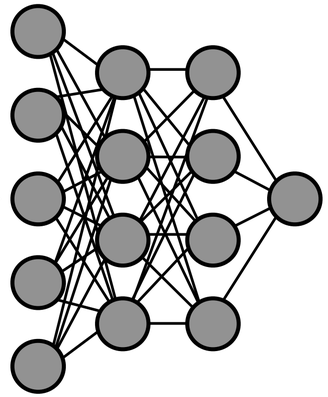
max log likelihood wrt ϕ

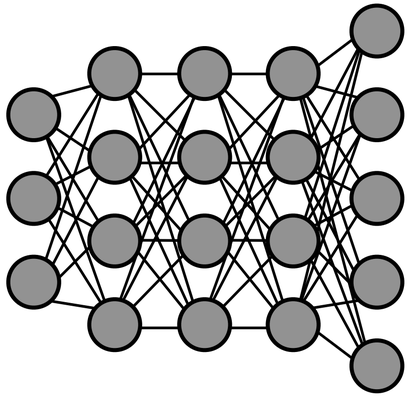
real image



discriminator P_ϕ

label: +1

noise



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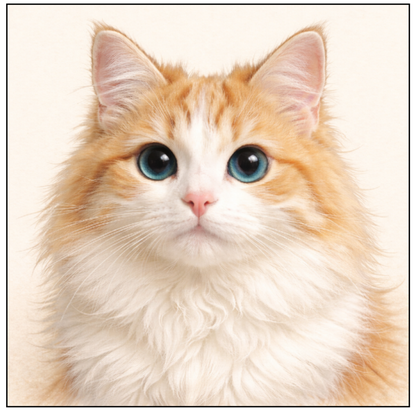

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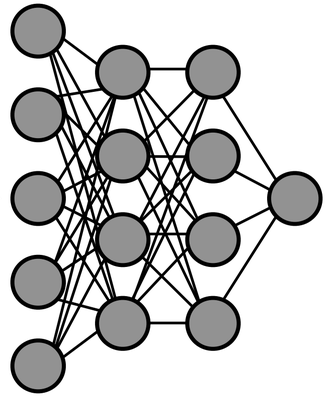
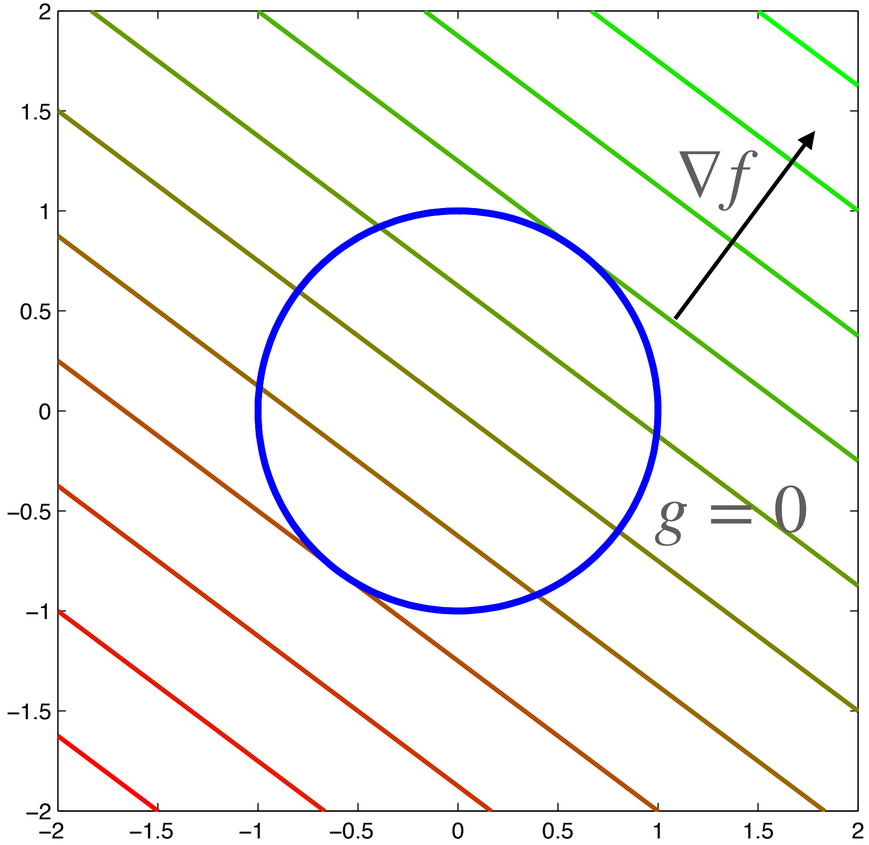


discriminator P_ϕ

label: –1

Geoff Gordon

Solving adversarial learning objectives



- For simple problems, we can find equilibria exactly
- E.g.: $\max_{x,y} f(x,y)$ s.t. $g(x,y) = 0$ where

$$f(x,y) = 6x + 8y$$

$$g(x,y) = x^2 + y^2 - 1$$

$$f(x, y) = 6x + 8y$$
$$g(x, y) = x^2 + y^2 - 1$$

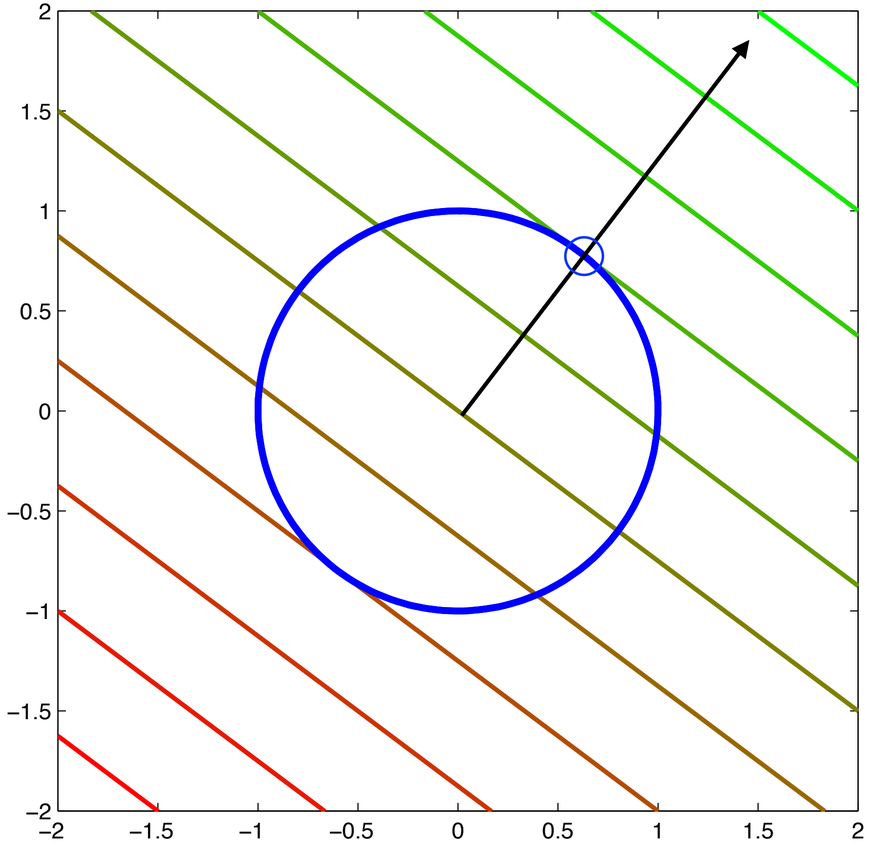
Construct and solve min-max problem

- Enforce equality with an adversary (Lagrange multiplier)
  - $\min_{x,y} \max_a L(x, y, a) = f(x, y) + ag(x, y)$
- At equilibrium, gradients are 0:

$$0 = \nabla_{x,y} L =$$

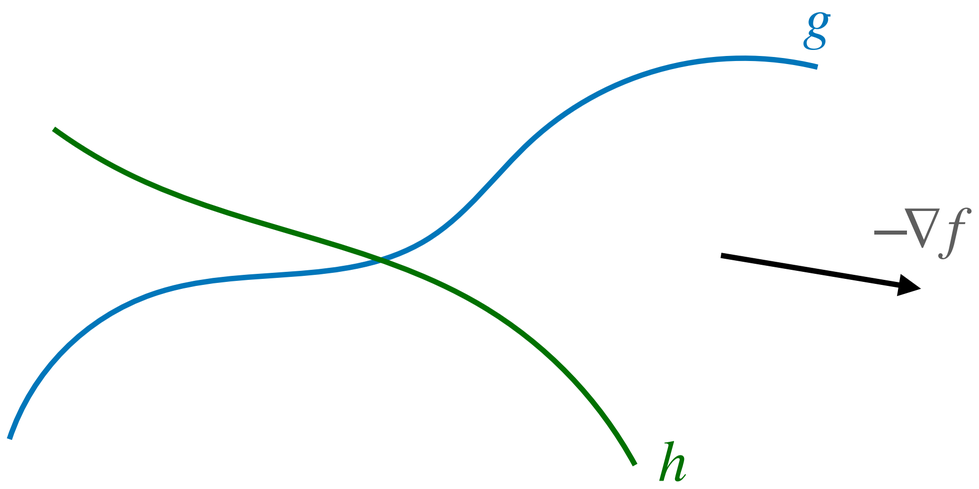
$$0 = \nabla_a L =$$

Solution



- So: (x, y) are a multiple of $(6, 8)$ and also lie on unit circle: must be $(\frac{3}{5}, \frac{4}{5})$

Multiple constraints



- We enforced an equality constraint by adding a single real-valued Lagrange multiplier
- It works equally well for multiple constraints: one multiplier per constraint

$$\max_{x,y} f(x,y) \text{ s.t. } g(x,y) = 0,\ h(x,y) = 0$$

$$\min_{x,y} \max_{a,b} L(x,y,a) = f(x,y) + ag(x,y) + bh(x,y)$$

- Interpretation: $a\nabla g(x,y)$, $b\nabla h(x,y)$, $-\nabla f$ are forces acting on (x,y) — at optimum, forces are in equilibrium

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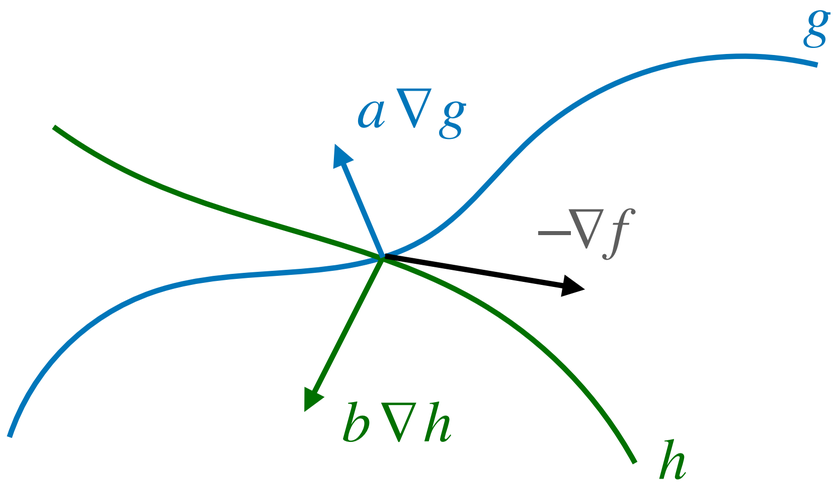

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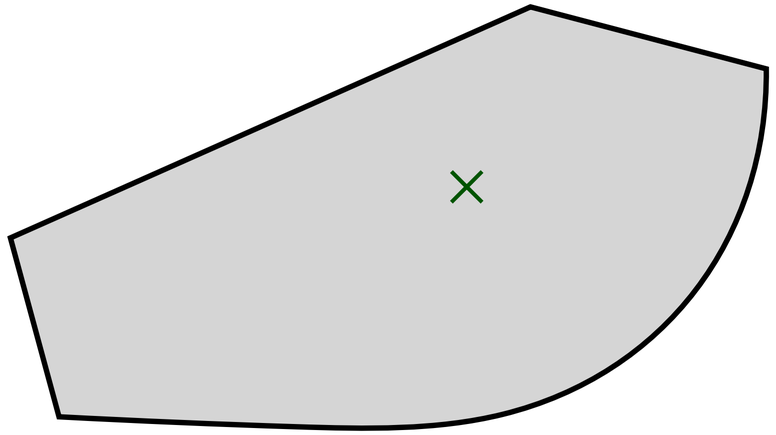
One-sided (inequality) constraints



- Constrain point x to lie in a convex set: use a Lagrange multiplier that is a multiple of the ***normal*** to the set at x
  - interpret as a force pushing x back into the set
  - only negative or zero multiples allowed: only push inward
- At a corner, there is a ***normal cone***, and any vector in that cone is a legal value for –multiplier
- Normal forces for all constraints must cancel at equilibrium

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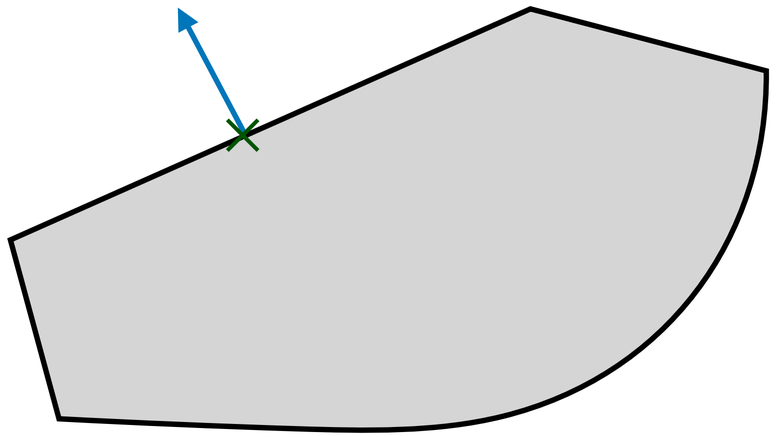

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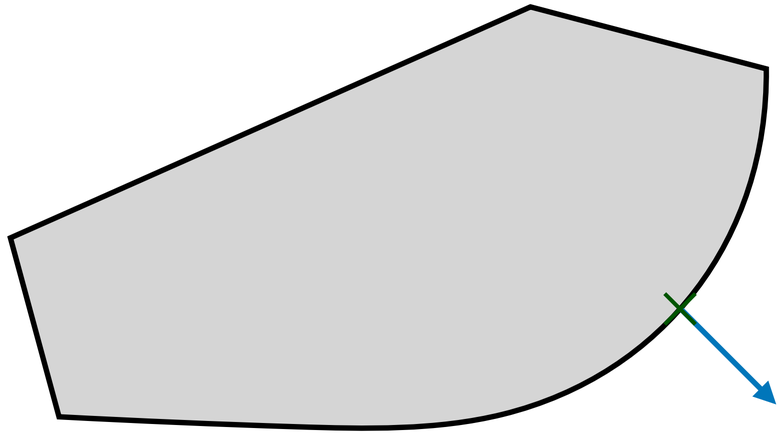

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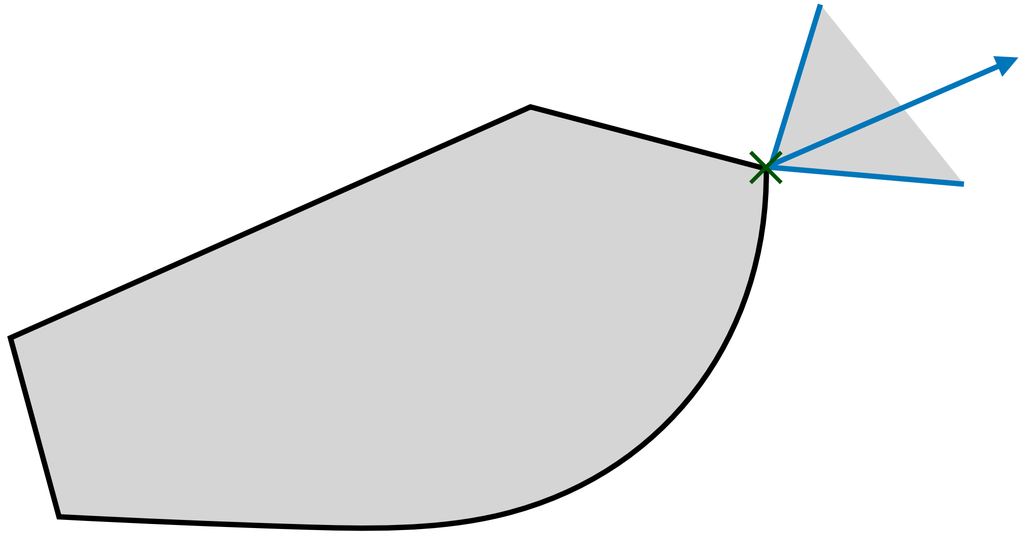

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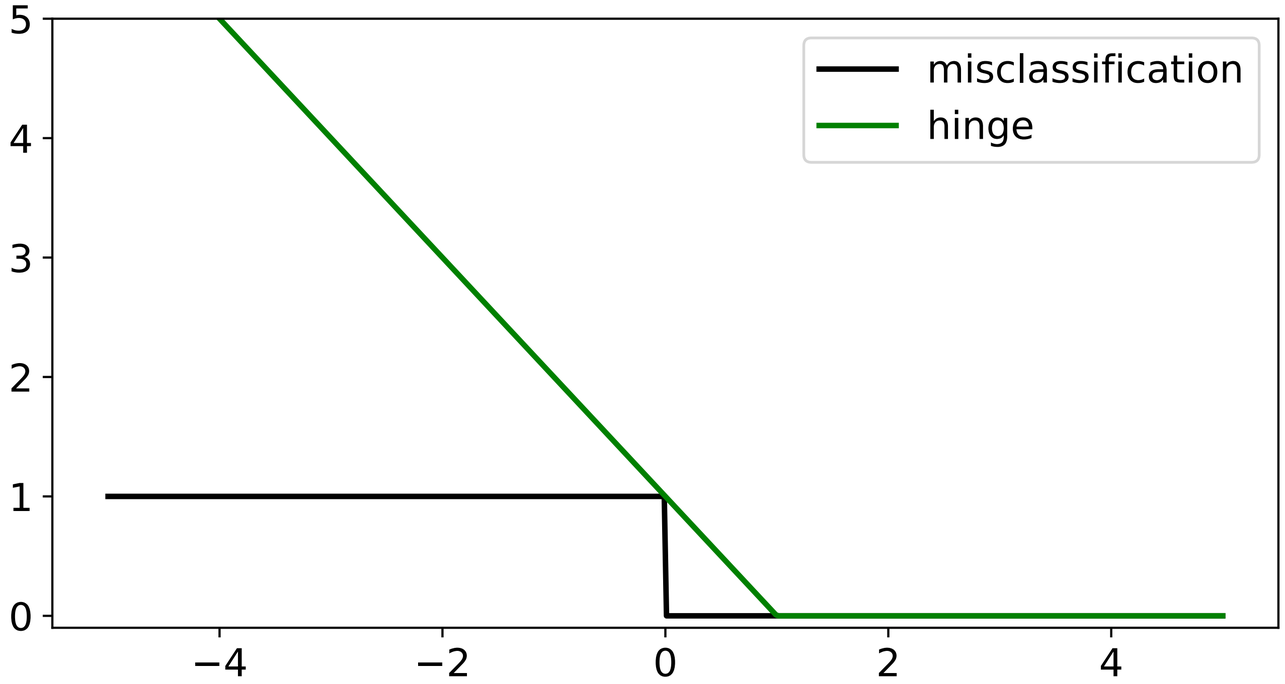
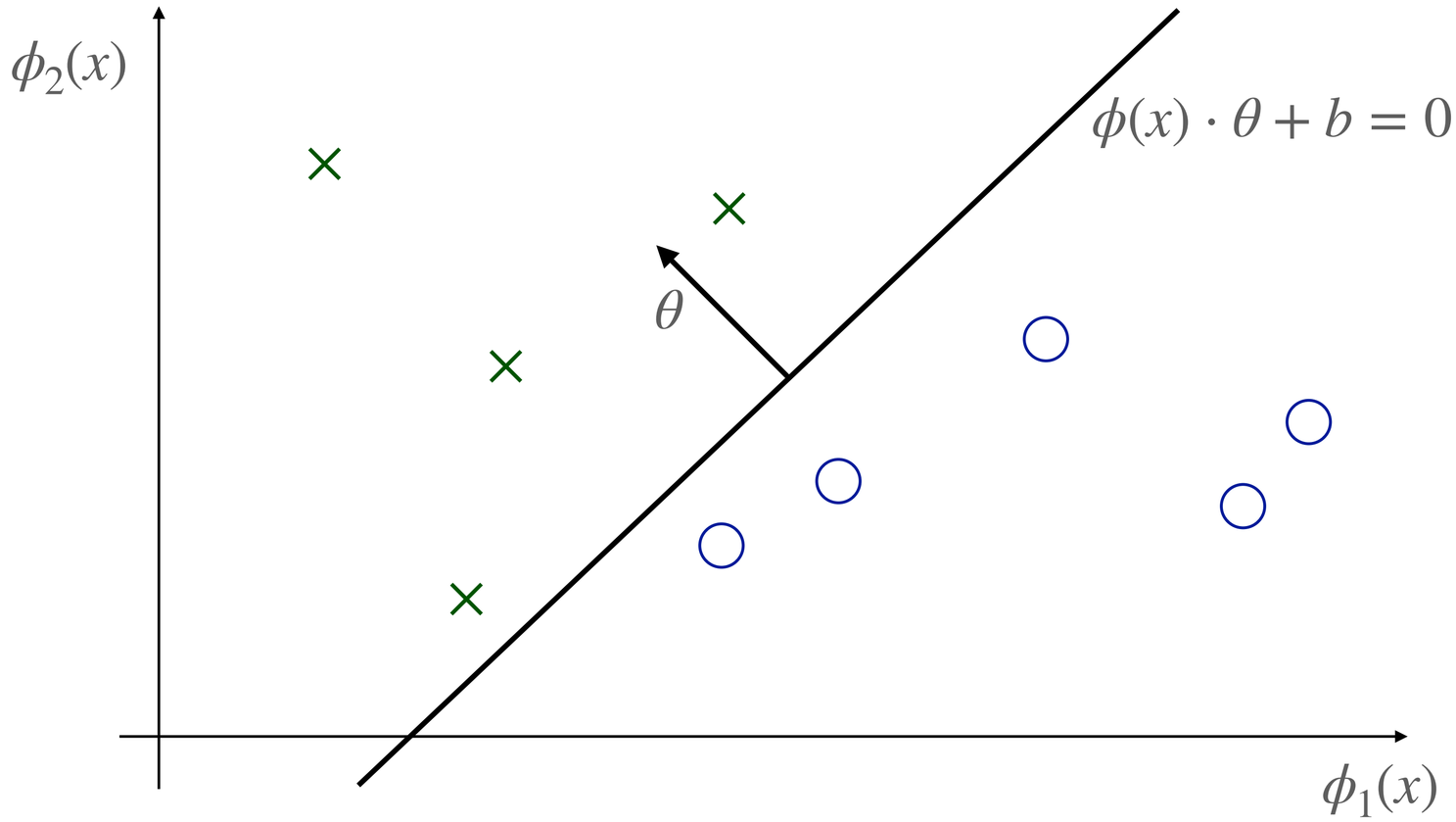
Example: classifier



$$\min_{f \in \mathcal{H}} L(f) = \sum_{i=1}^{N} \ell(y^{(i)} f(x^{(i)}))$$

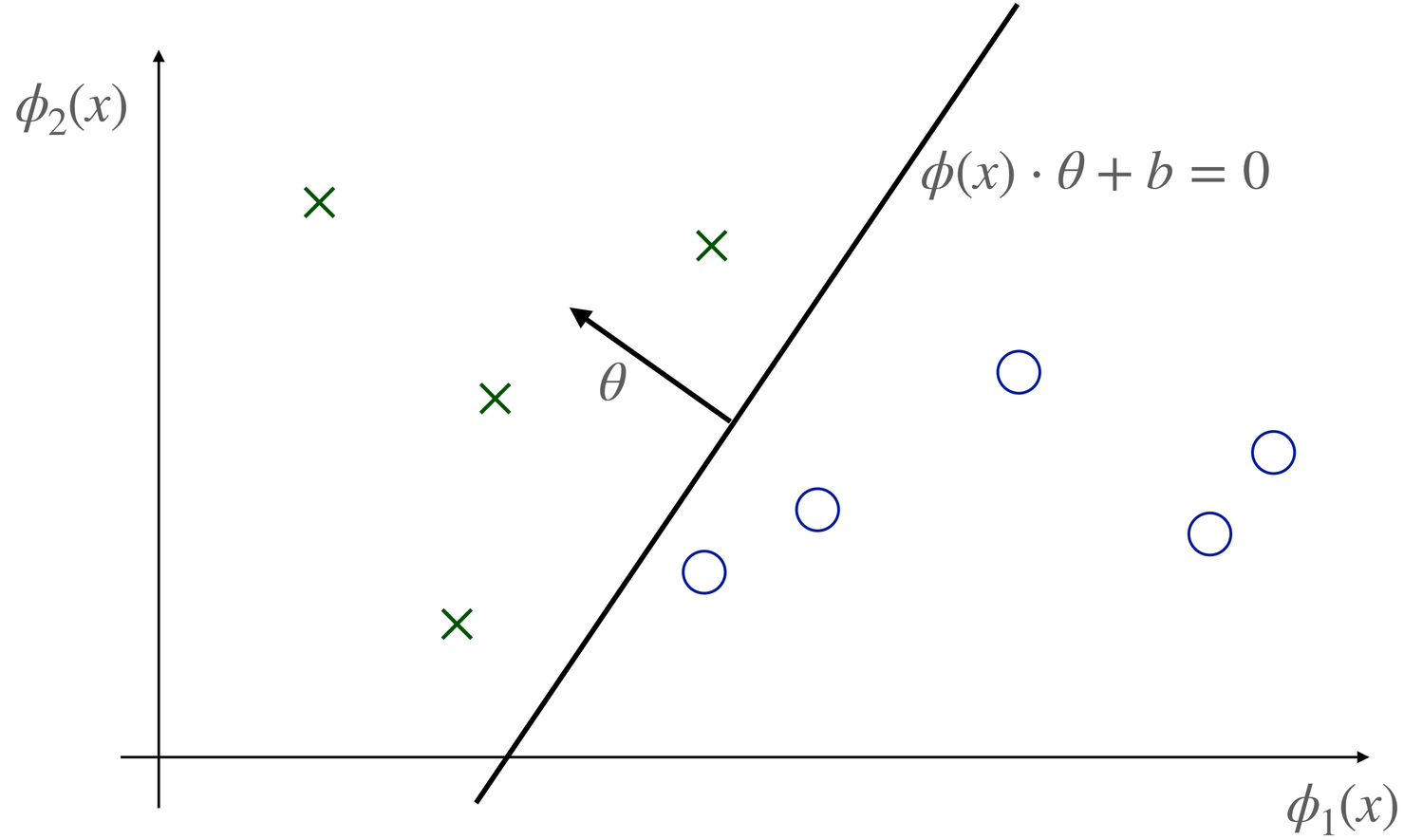
- choose hinge loss as bound: $\ell(z) = \max(0, 1 - z)$
- minimizer wants $f(x^{(i)}) \geq 1$ for +ve examples, $f(x^{(i)}) \leq -1$ for –ve examples

Linear classifier



- Linear $f(x) = \phi(x) \cdot \theta + b$
  - note intercept b (not shown in picture)
- Decision boundary is where $\phi(x) \cdot \theta + b = 0$

Linear classifier



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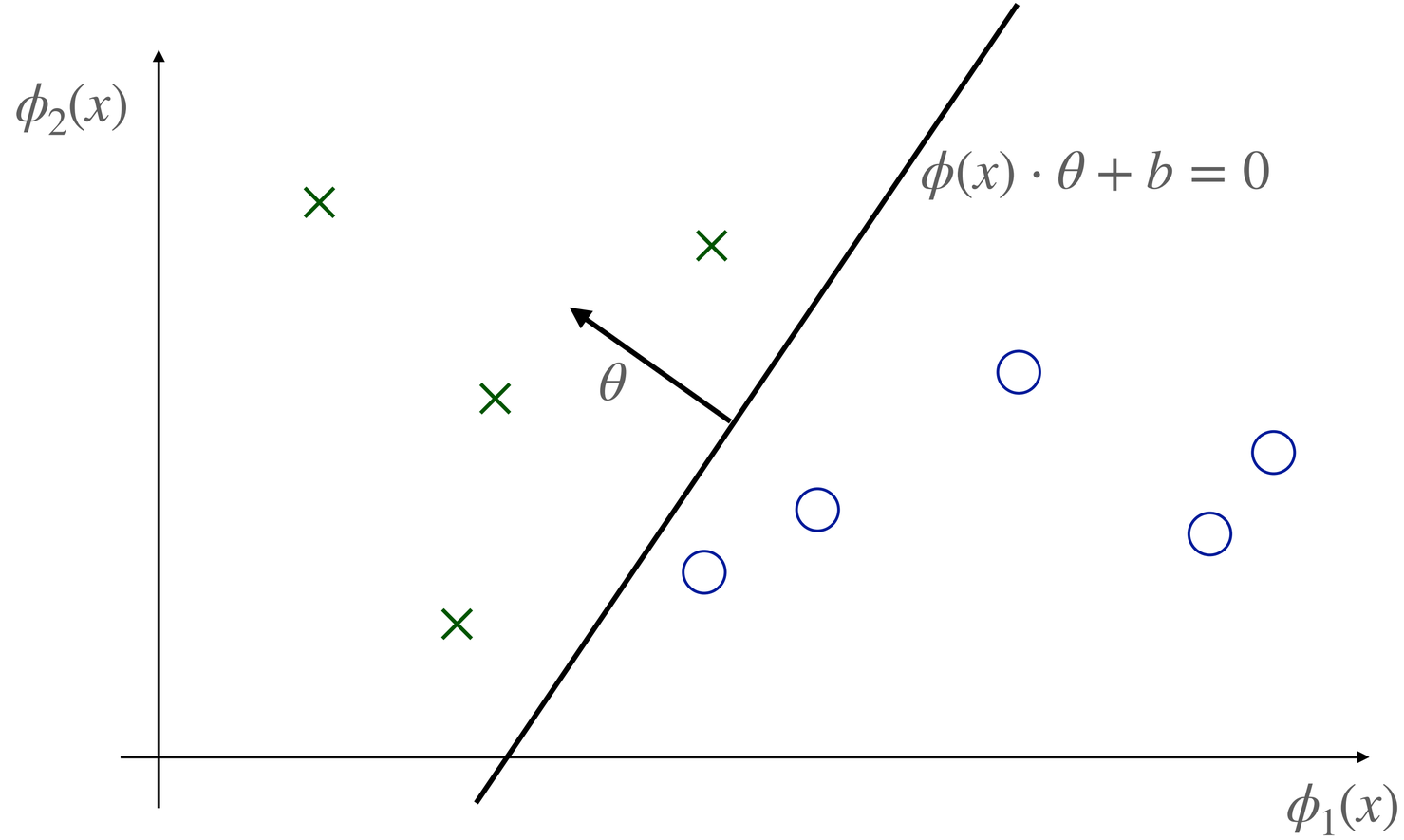
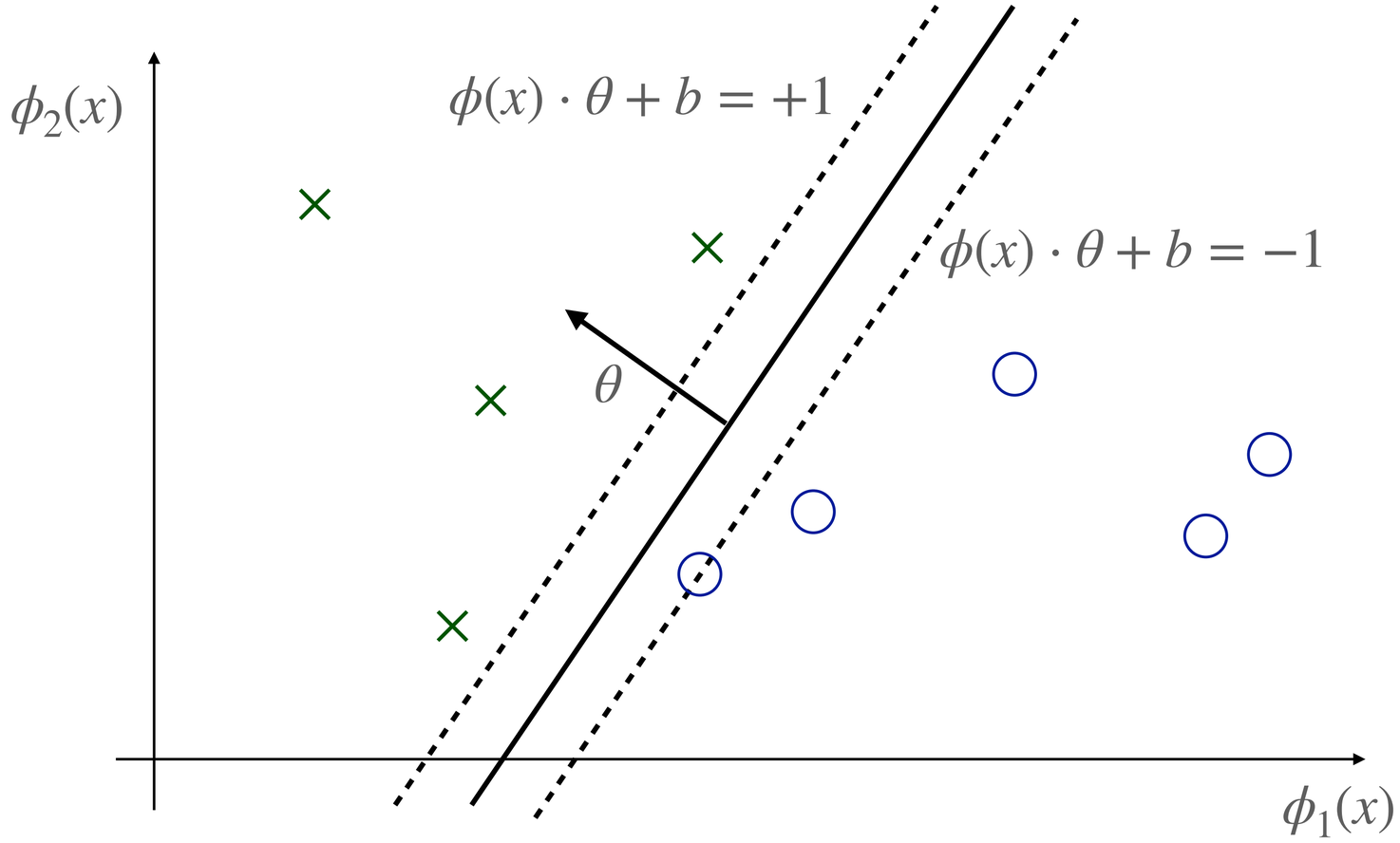
- Decision boundary is where $\phi(x) \cdot \theta + b = 0$

Margin



- Hinge loss starts increasing when $\phi(x) \cdot \theta + b = 1$ (positive examples) or -1 (negative examples)
  - boundaries are called ***margins***
- Scaling θ changes location of margins but not boundary

Margin



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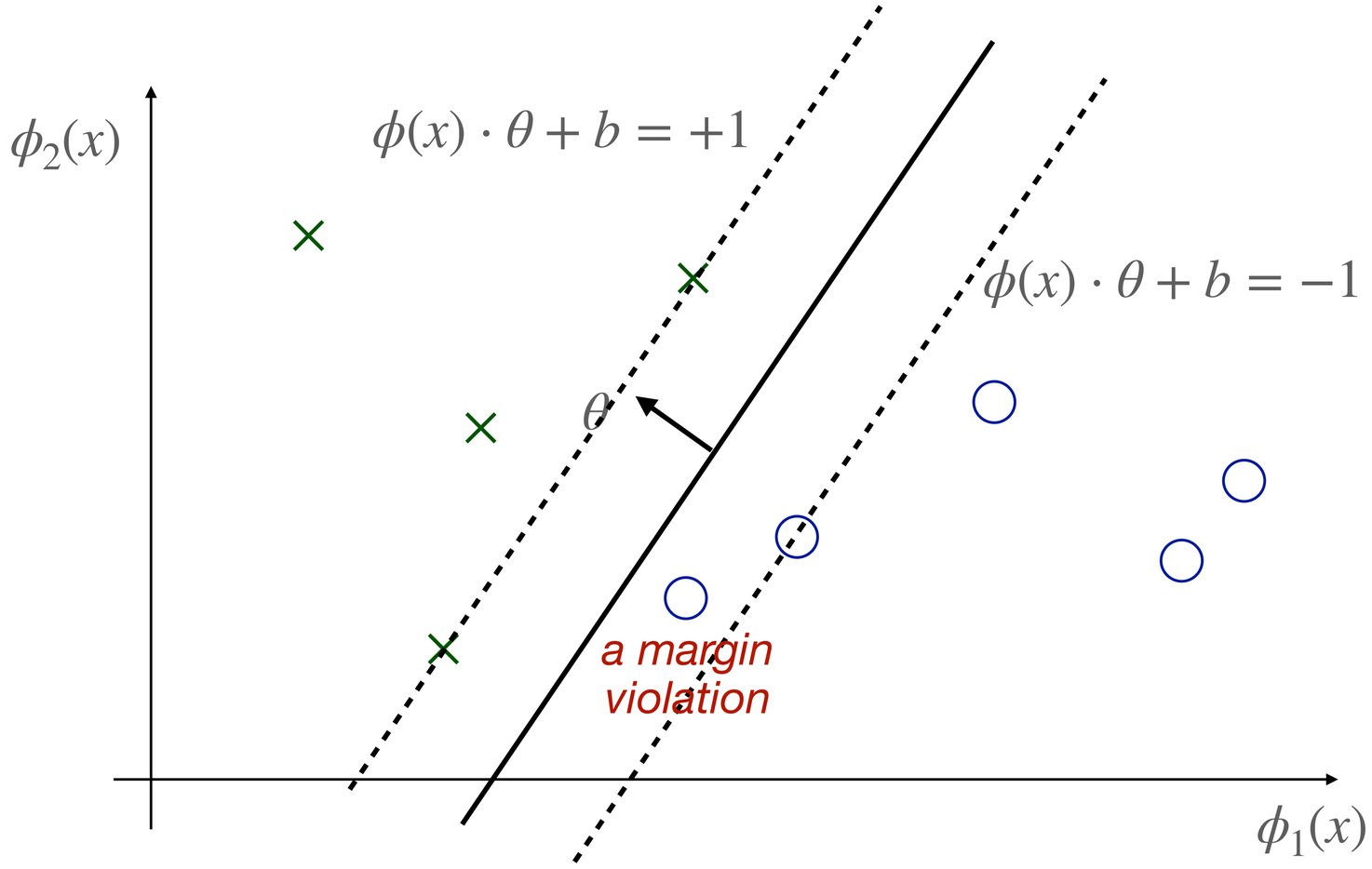

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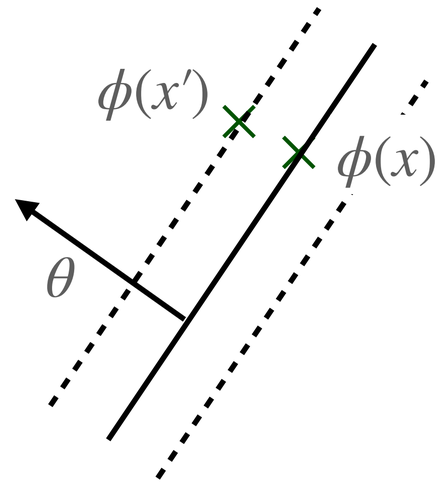
Distance to margin

confusingly, *margin* can mean both the dashed line itself and the distance between the dashed line and decision boundary



- We can calculate distance from the decision boundary to the margin: an example with $\phi(x) \cdot \theta + b = 0$ is on the boundary, and one with $\phi(x') \cdot \theta + b = 1$ is on the margin. Subtracting, $(\phi(x') - \phi(x)) \cdot \theta = 1$. Shortest distance is if $\phi(x') - \phi(x)$ is parallel to θ: i.e., equal to $a\theta$ for some $a \in \mathbb{R}$. Substituting, $a\theta \cdot \theta = 1$. Solving,

$$a = \frac{1}{\|\theta\|^2} \text{ and the distance is } \|a\theta\| = \frac{1}{\|\theta\|}$$

SVM

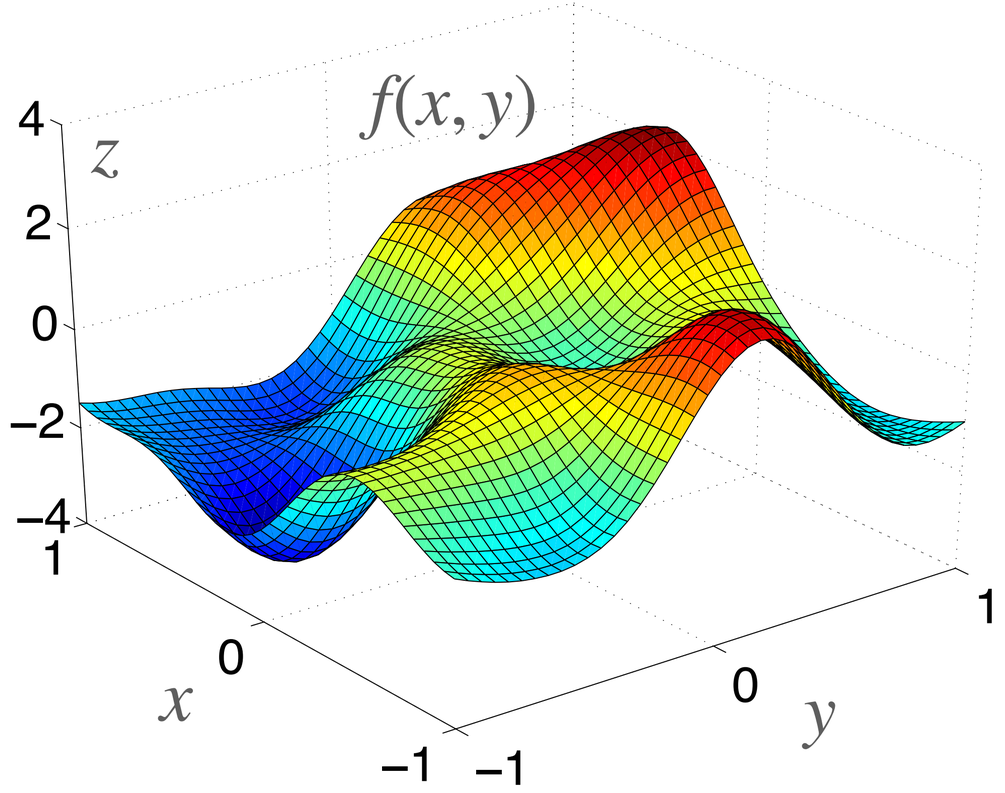
- For a linearly separable dataset, without regularization, we'll just scale up θ so that all points are outside margin
- To prevent this, regularize:

$$\min_{\theta,b} C \sum_{i=1}^{N} \ell(y^{(i)}(\phi(x^{(i)}) \cdot \theta + b)) + \frac{1}{2}\|\theta\|^2$$

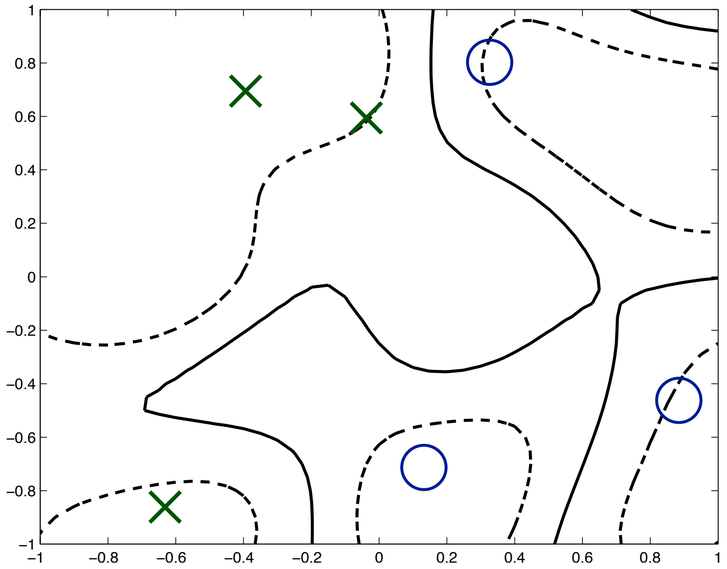
  - make θ small (distance to margin $\frac{1}{\|\theta\|}$ large) while still getting low total hinge loss ℓ
- Constant $C > 0$ weights loss vs. regularizer
  - large C prioritizes ℓ: larger θ, fewer margin violations
  - C near 0 prioritizes regularizer: smaller θ at cost of more margin violations
- This is a (linear) ***support vector machine*** or ***SVM***

Nonlinear SVM

discrimination function



margin

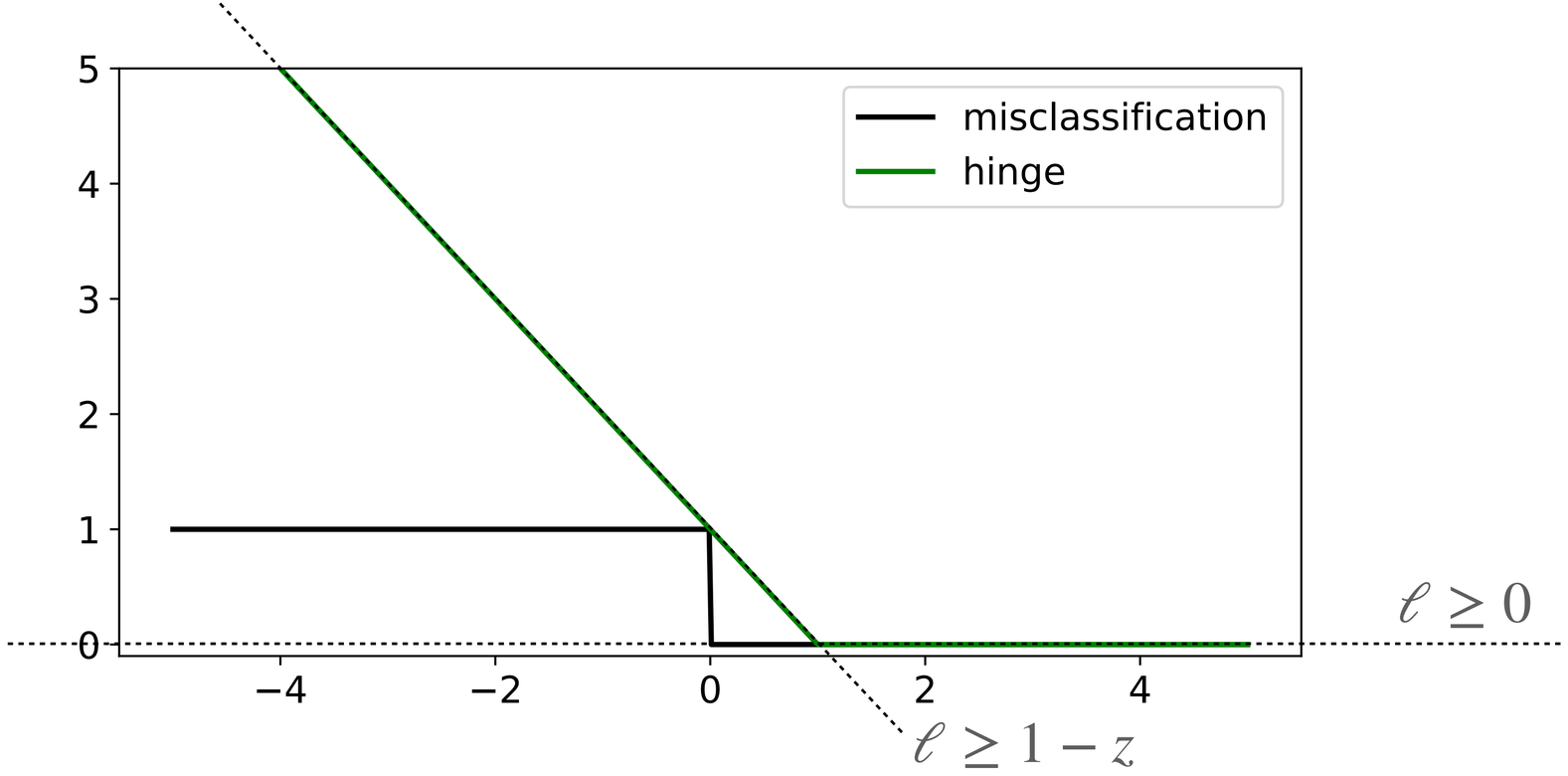


- We can also define a nonlinear SVM (more on that soon!)

Why maximize distance to margin?

- It's another way of limiting the complexity of our hypothesis class
- Just like
  - Haussler bound limits number of distinct hypotheses
  - VC bound limits number of hypotheses that are distinct *on our given set of inputs* $x^{(i)}$
- We can make a margin-based bound: there aren't that many ways we can fit a fat margin in between datapoints
  - wrinkle: margin bound needs to condition on our dataset
  - i.e., we can't say ahead of time that an SVM will generalize; but if we optimize and observe that we got a large margin, we can be confident of good generalization

Solving the linear SVM



- Objective: $\min_{\theta,b} C \sum_{i=1}^{N} \ell(y^{(i)}(\phi(x^{(i)}) \cdot \theta + b)) + \frac{1}{2}\|\theta\|^2$
- Rewrite ℓ: we know $\ell \geq 0$ and $\ell \geq 1 - z$
  - and since we're minimizing ℓ, we can just enforce these constraints, and the optimizer will make one of them tight

Quadratic program for SVM

$$\min_{\theta,b,\ell_i} C\sum_{i=1}^{N}\ell_i + \frac{1}{2}\|\theta\|^2 \text{ s.t.}$$

$$(\forall i)\ \ell_i \geq 0$$

$$(\forall i)\ \ell_i \geq 1 - y^{(i)}(\phi(x^{(i)}) \cdot \theta + b)$$

- We've eliminated the nonlinear hinge loss function $\ell(z)$, replacing it by extra variables ℓ_i ($i = 1 \ldots N$) and linear inequality constraints
- Minimizing a quadratic objective under linear constraints is a *quadratic program*; this one is a *convex* QP because the objective is convex for minimization
  - in fact there's a unique globally optimal θ
  - and there are fast algorithms for finding it, if dimension of θ and $\phi(x^{(i)})$ is not too high (QP size $\propto$ # dims $\times N$)

Quadratic program for SVM

pay a penalty for margin violations ↘ ↙ *maximize distance to margin*

$$\min_{\theta,b,\ell_i} C\sum_{i=1}^{N} \ell_i + \frac{1}{2}\|\theta\|^2 \text{ s.t.}$$

$$(\forall i)\ \ell_i \geq 0 \quad \leftarrow \textit{don't worry if we're on good side of margin}$$

$$(\forall i)\ \ell_i \geq 1 - y^{(i)}(\phi(x^{(i)}) \cdot \theta + b) \leftarrow \textit{classify each example correctly or measure margin violation}$$

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Reformulate the SVM

- What if dimension of $\phi(x)$ is too high?
- We can use adversarial learning to reformulate the SVM
- The size of the QP will become ***independent*** of the dimension of $\phi(x)$
  - but unfortunately will be proportional to N^2 not N
  - a win if $N \ll$ # dims of ϕ
  - in a bit, we'll even use functional ML to handle infinite-dimensional features $\phi(x^{(i)})$

Dual SVM

$$\min_{\theta,b,\ell_i} C\sum_{i=1}^{N}\ell_i + \frac{1}{2}\|\theta\|^2 \text{ s.t.}$$

$$(\forall i)\ \ell_i \geq 0$$

$$(\forall i)\ \ell_i \geq 1 - y^{(i)}(\phi(x^{(i)})\cdot\theta + b)$$

- Last constraint is the annoying one:
  - [complicated function]$_i \leq 0$ for all i
  - i.e., [complicated function] has to be in $\mathbb{R}^N_{\leq 0}$
  - introduce an adversary α that takes values in the normal cone of $\mathbb{R}^N_{\leq 0}$
  - α is also called a Lagrange multiplier or a dual variable

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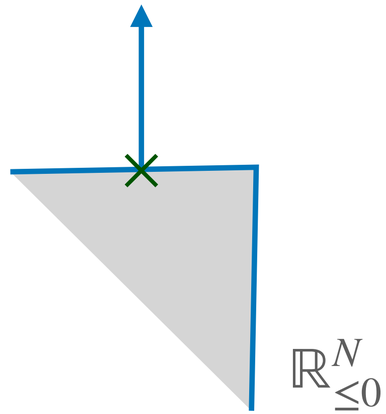

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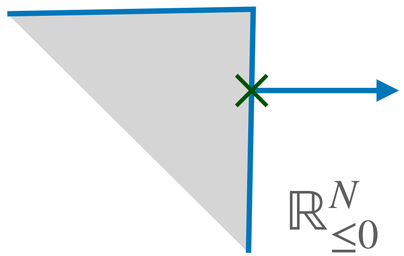

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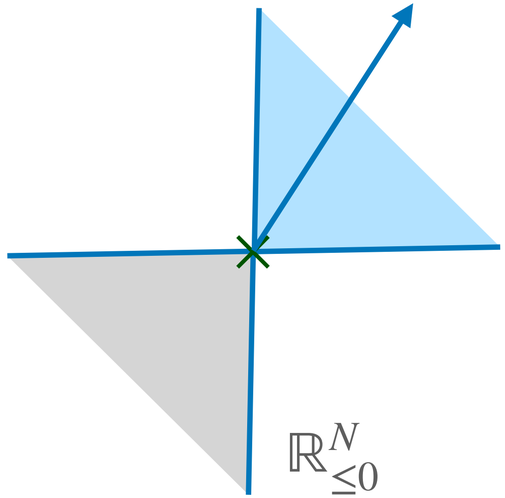

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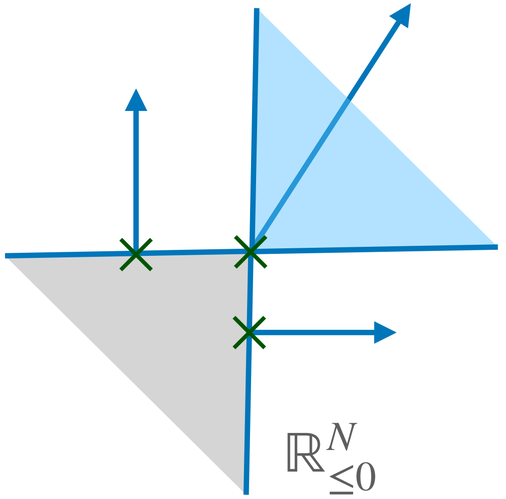
Complementary variables

- Normal cone takes different shapes depending on
  $s_i = 1 - y^{(i)}(\phi(x^{(i)}) \cdot \theta + b) - \ell_i$
  - it's always a subset of $\mathbb{R}^N_{\geq 0}$
  - if $s_i < 0$ then we're not on the boundary in dimension i, and α_i must be 0
  - and if $\alpha_i > 0$ it means we must be on the boundary in dimension i
- Write constraints compactly:
  - $\alpha \geq 0$ componentwise
  - $s \leq 0$ componentwise
  - each $\alpha_i s_i = 0$: at most one of α_i or s_i can be nonzero
  - equivalently $\alpha^\top s = 0$: since each $\alpha_i s_i$ term is ≤ 0, sum can only be zero if all are zero



called ***complementarity***

Dual SVM

$$\max_{\alpha_i,\theta} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \left\| \sum_{i=1}^{N} \alpha_i y^{(i)} \phi(x^{(i)}) \right\|^2 \text{ s.t. } 0 = \sum_{i=1}^{N} \alpha_i y^{(i)}$$

$$\text{where } (\forall i)\ 0 \le \alpha_i \le C$$

- Introducing the dual variables α_i leads to a min-max objective (not shown)
- We can then analytically eliminate θ, b, ℓ_i to get the ***dual SVM*** quadratic program (above)
- In the process we derive $\theta = \sum_{i=1}^{N} \alpha_i y^{(i)} \phi(x^{(i)})$, which lets us recover the optimal classifier from the dual α_is
  - intercept b is then a 1-d optimization of a piecewise linear objective: similar computation to finding a median

Interpreting the dual variable

- Recall $\alpha_i s_i = 0$ where s_i is constraint RHS for example i
  - If $\alpha_i > 0$ then constraint must be tight: example i is on margin (if $\ell_i = 0$) or margin violation (if $\ell_i > 0$)
  - if example i is strictly on good side of margin (constraint is loose), then $\alpha_i = 0$
  - so $\alpha_i > 0$ picks out examples that are actively constraining θ: the ***support vectors***
  - bigger α_i means the example is affecting θ more strongly
  - smaller α_i means the example has less influence
  - $\alpha_i = 0$ means *no* influence: we could delete all non-support-vector examples and θ wouldn't change
  - sparsity is common: often # support vectors $\ll N$

SVM summary

- If we train a linear classifier using the hinge loss, we can optimize via a convex quadratic program
- Adversarial learning (duality) allows us to reformulate:
  - original (primal) program's size depends on dimensionality of feature vector $\times$ number of examples
  - dual program's size depends on (number of examples)^2 and is completely independent of feature dimension
  - we can solve whichever is smaller and recover best θ, b
- We can interpret both versions:
  - primal: maximize the margin while avoiding too many margin violations
  - dual: discover which examples are support vectors (actively constrain the decision boundary because they are on the margin or violate it)