Ya gotta make it obvious

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A bit of background…

- I'm retooling as a machine learning droid after an entire career in parsing and programming language implementation
  (you might know me as "the ANTLR guy")
- Since I'm no longer subject to the paper count treadmill, I'm exploring less traditional scholarly work, such as creating state-of-the-art visualizations and animations to explain machine learning concepts and models: https://explained.ai/
- My mission is to explain complex topics deeply, but in the simplest possible way, and to build useful libraries to help the research and education community
- *My niche is what industry can't justify and academy doesn't value*

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What's wrong w/traditional academic output?

- The goal of academic research papers and instruction is to transmit ideas, but…
- Peer review and our egos often work against this goal because they are the enemy of simplicity and clarity
- We fear that simplicity implies small research contribution and we also want to impress our audience with our brilliance
- Therefore, we "math it up" or simply don't bother spending time to make our techniques or results clear
- We should value simple and clear expositions most of all, for both large and small contributions, even if it's lots of extra work
- Try to illuminate not impress!

What's wrong with articles and lectures?

- It's frustrating trying to learn new concepts in machine learning
- There is some excellent content on the net, but most of it is the same superficial mostly-correct article rehashed 10^5 times
- There are lots of pain points that don't seem to bother people, or perhaps they think it's the best we can do; e.g., debugging and visualization aids can be primitive
- In contrast, academic papers are correct but usually too dense to include examples and don't allow dynamic content like animations and video
- What we need: correct, deep, and obvious (as possible)

Advice on achieving "correct, deep, and obvious"

1. Seek a deep understanding of concepts
   - Ask why or how something works; be able to reproduce the technique
   - W/o depth, we can't get to the essence, to zero in on the critical idea
   - W/o depth, we can't strip away any mysticism (I'm talkin to you neural nets!)
   - Can you describe the essence in one key phrase or sentence? 🔑
2. Target the human visual cortex in your artifacts
3. Rederive everything and baby step the audience to the solution; don't start with the final math solution, for example
4. You can't build what you can't imagine; don't limit yourself by what's possible or what you know how to build; engage your audience!
5. Sometimes you are right and everyone else is wrong

Some examples following this advice

Explaining gradient boosting (regression)

- Start by isolating the essence of boosting; boil it down!
- Next, design a visualization that clearly shows the key bits
- Boosting is just the addition of an initial "drive" f_0 plus a series of imprecise "putts" Δ_i

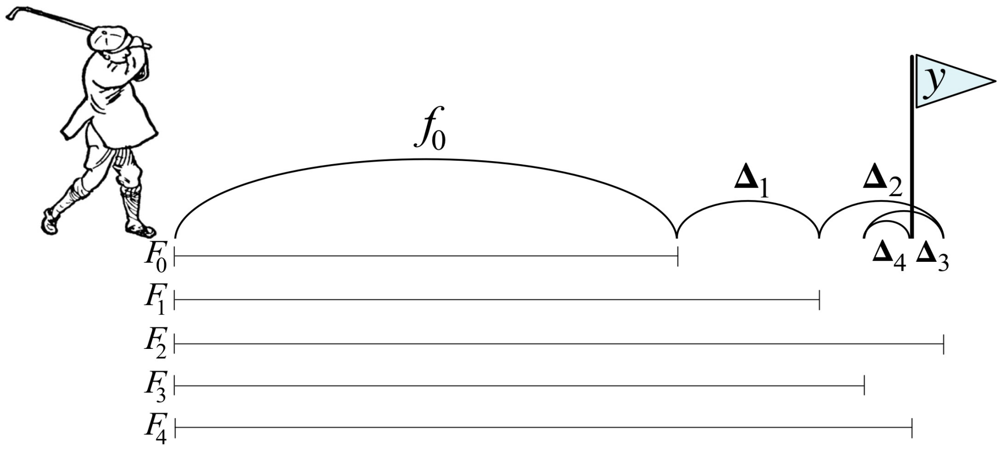

Diagram from https://explained.ai/gradient-boosting/index.html
but golfer clipart from http://etc.usf.edu/clipart/

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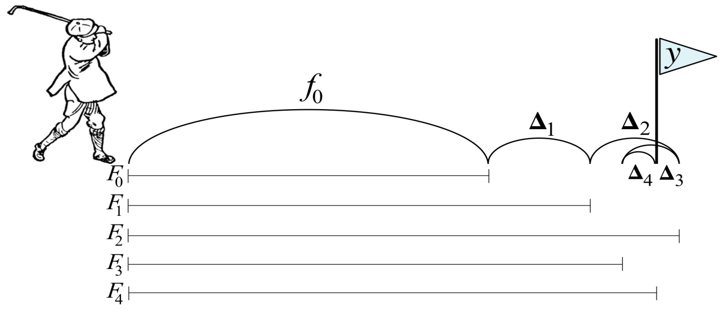
Explaining gradient boosting (regression)

- **Then**, with this intuition, show the concise equation that embodies the process:

$$\begin{aligned}\hat{y} &= f_0(\mathbf{x}) + \Delta_1(\mathbf{x}) + \Delta_2(\mathbf{x}) + \ldots + \Delta_M(\mathbf{x}) \\ &= f_0(\mathbf{x}) + \sum_{m=1}^{M} \Delta_m(\mathbf{x}) \\ &= F_M(\mathbf{x})\end{aligned}$$



Don't start with the math!
The math is the condensation of an inventor's intuition
The inventor didn't start with the answer; why should our audience have to?

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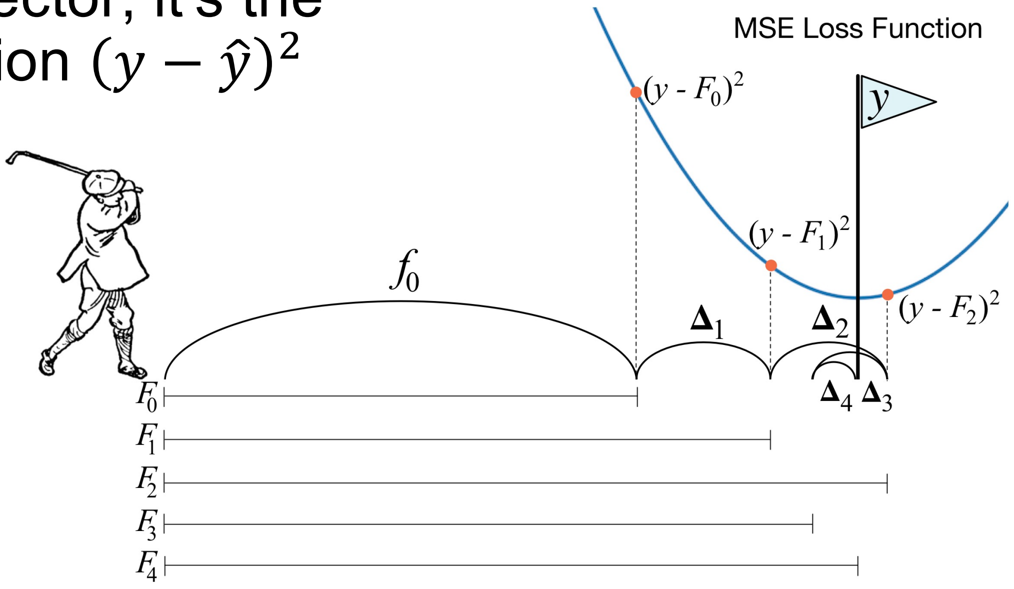
While we're at it…
GBMs: Gradent descent in prediction space

- Clarifying a common fuzzy detail
- Difference $y - \hat{y}$ is not just a vector; it's the gradient of the MSE loss function $(y - \hat{y})^2$
- Chasing the difference vector performs MSE gradient descent in prediction space



See https://explained.ai/gradient-boosting/descent.html#sec:3.2 for more details

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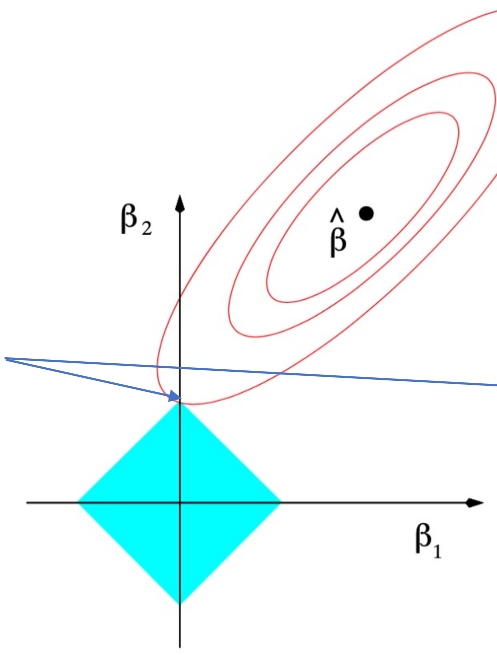
Just because it's visual doesn't mean it's effective

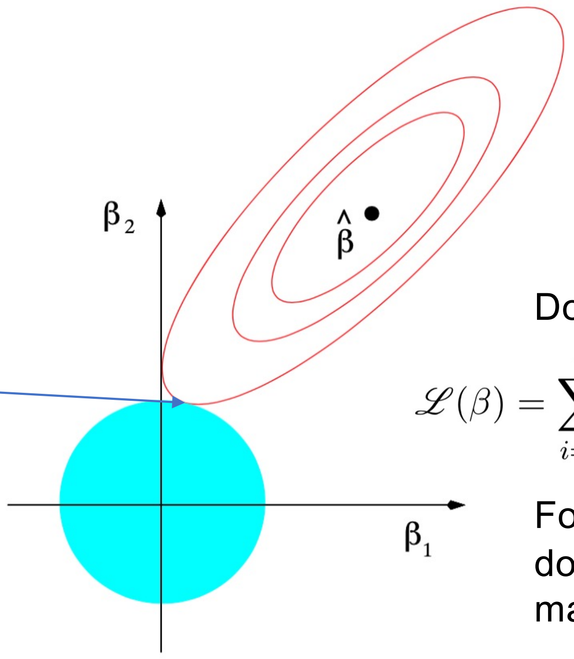
Viz meant to help explain L1 vs L2 regularization and why L1 encourages zero coefficients but L2 does not

(ESL is a great book written by brilliant statisticians, but these visualizations never helped me)

Why here?



L1 regularization (lasso)



L2 regularization (ridge)

Don't show this math first:

$$\mathscr{L}(\beta) = \sum_{i=1}^{n}(y^{(i)} - (\mathbf{x}'^{(i)} \cdot \beta))^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

For one thing, the pictures don't correspond to that math!!!

Fig 3.11, Page 71 Elements of Statistical Learning

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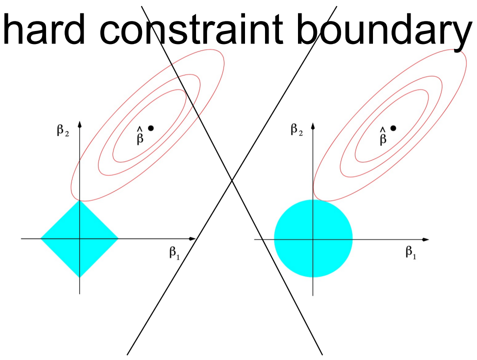
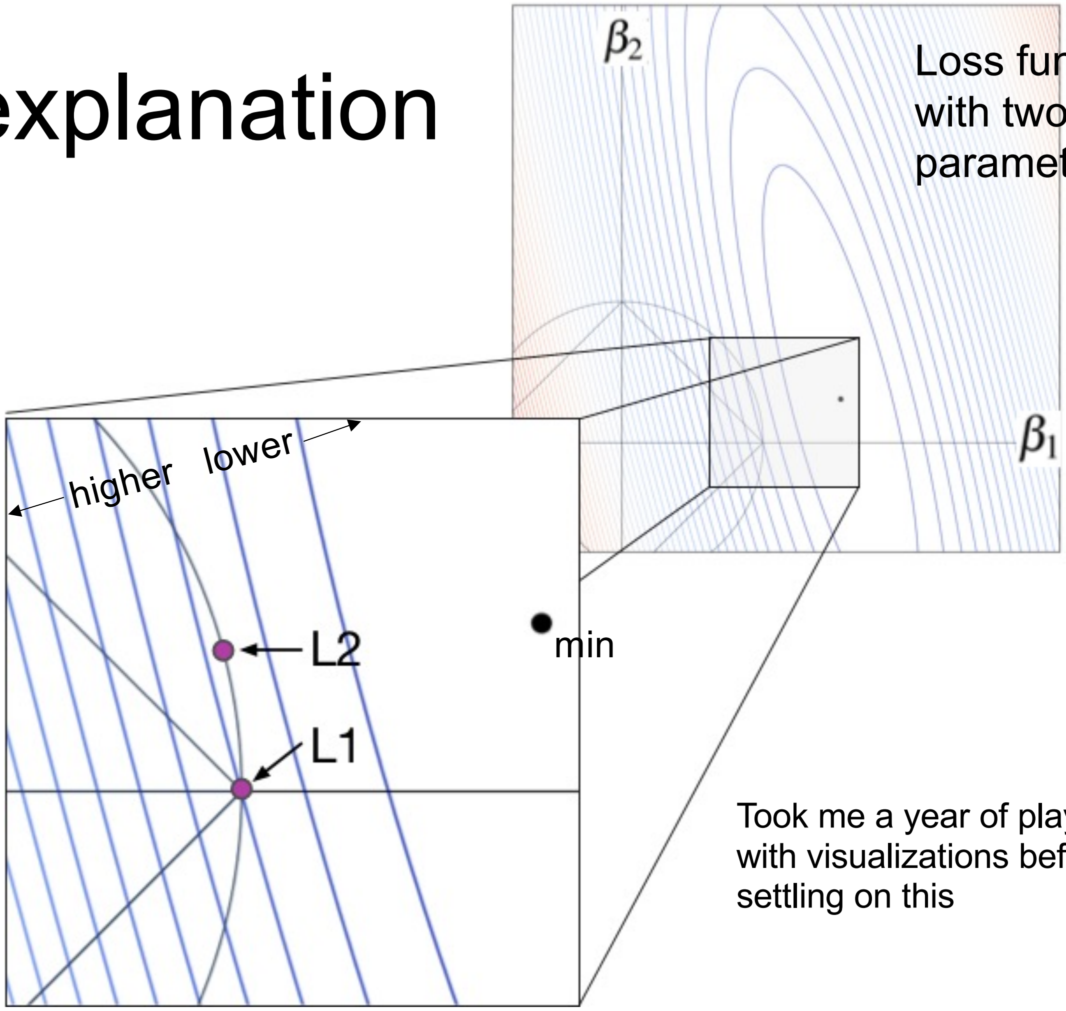
Better L1 vs L2 explanation

- Simple visual proof: Any movement of (β_1, β_2) away from purple L1 dot at $\beta_2 = 0$ increases the loss
- Left of any contour line is higher loss
- To shift away from 0, we'd need to rotate loss function contour lines to be more parallel with L1 hard constraint boundary





Loss function with two parameters

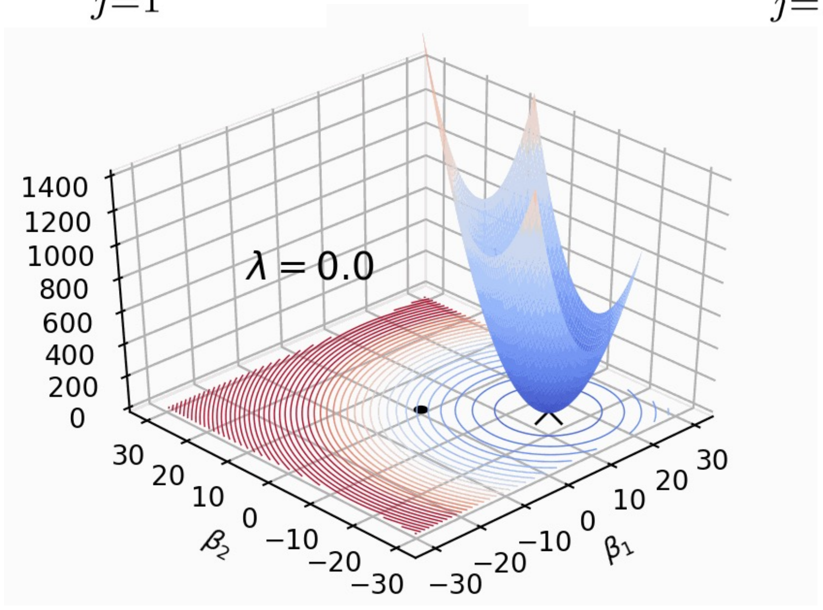
Took me a year of playing with visualizations before settling on this

From https://explained.ai/regularization/index.html

Sometimes animations and 3D help

- We use **hard constraint** regions conceptually but **soft constraints** to implement
- Increasing λ increases penalty at any (β_1, β_2) and shifts loss point towards the origin
- 3D animations are painful to build but illuminating

$\mathscr{L}(\beta)$ s.t. $\sum_{j=1}^{p} \beta_j^2 \le t$ becomes $\mathscr{L}(\beta) + \lambda \sum_{j=1}^{p} \beta_j^2$



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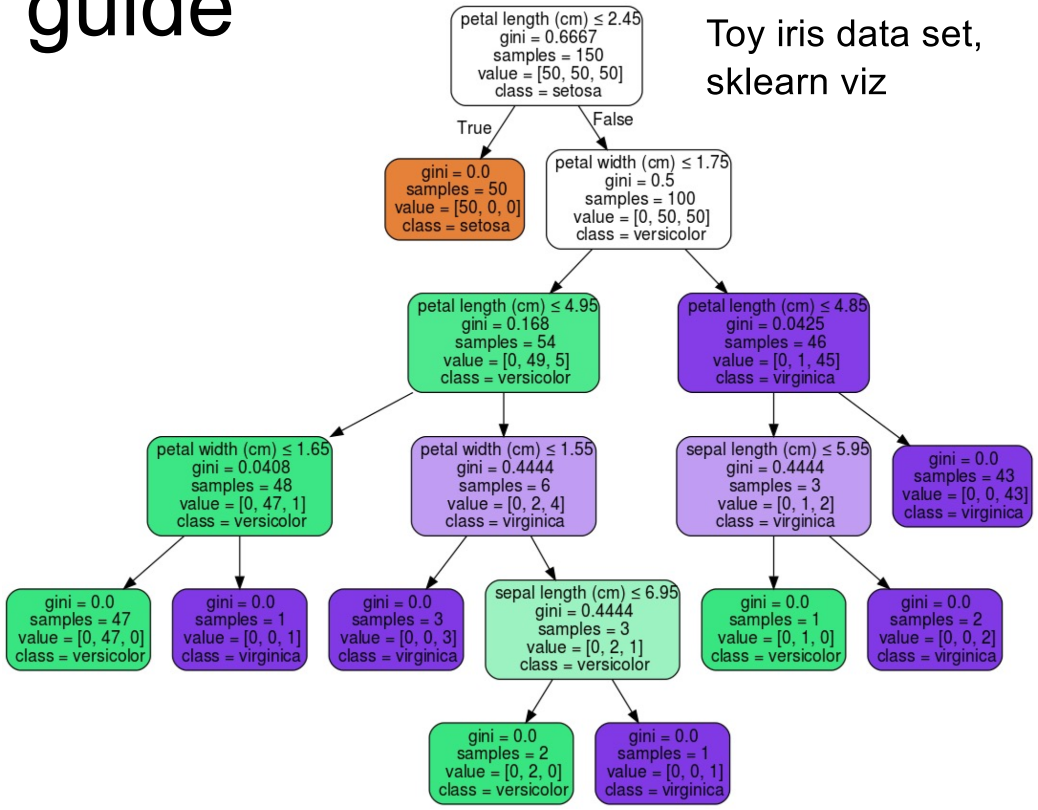
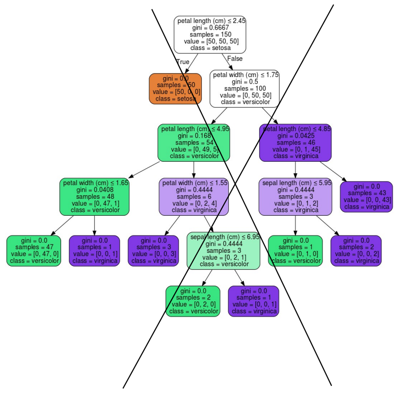
Let your imagination and deep understanding be your guide

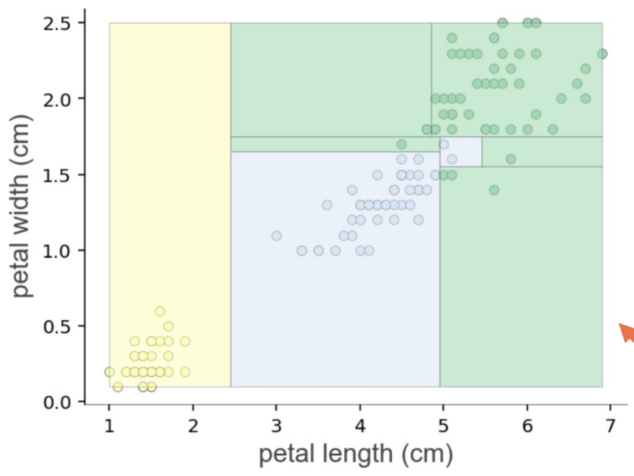
- Decision trees tesselate feature space into regions of feature space according to purity of target y; each node partitions a single var at a specific value
- Consider sklearn's viz, which shows tree structure, but that's not what we really care about
- I have to think too hard here; decisionmaking is not obvious
- Why were those split vars/values chosen? What do colors mean?



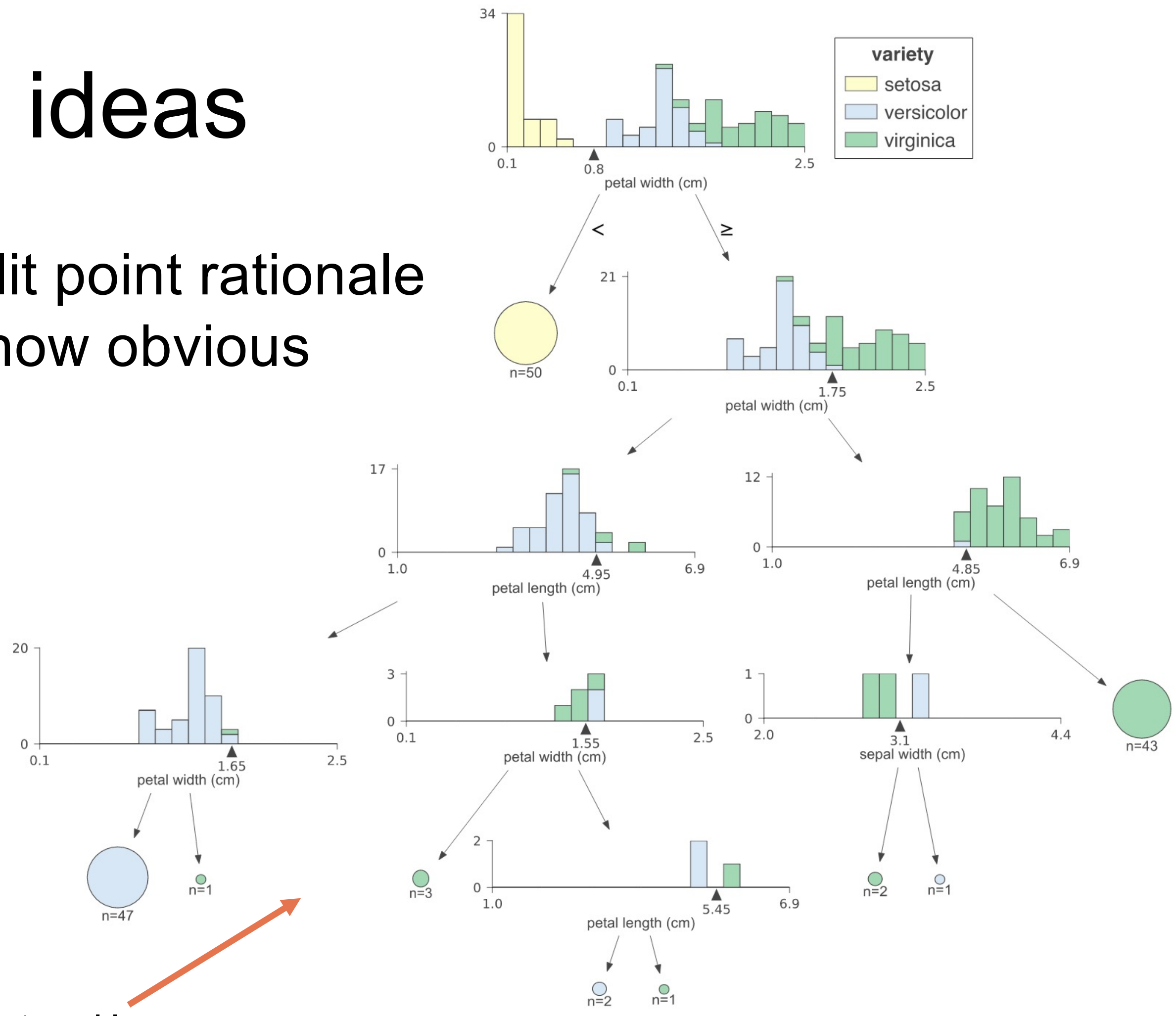
Toy iris data set, sklearn viz

Illustrate the key ideas





Split point rationale is now obvious



Effect How

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See https://explained.ai/decision-tree-viz/index.html

Debugging matrix algebra is not obvious

We often get less than helpful exception messages:

```
h_ = torch.tanh(Whh_ @ (r*h) + Uxh_ @ X.T + bh_)
```

C++?

```
RuntimeError: size mismatch, m1: [764 x 256], m2: [764 x 200] at
/tmp/pip-req-build-as628lz5/aten/src/TH/generic/THTensorMath.cpp:41
```

It's not clear why/where expression failed; I still have to think hard

We need operator and operands; TensorSensor generates:

```
Cause: @ on tensor operand Uxh_ w/shape [764, 256]
and operand X.T w/shape [764, 200]
```

See https://explained.ai/tensor-sensor/index.html

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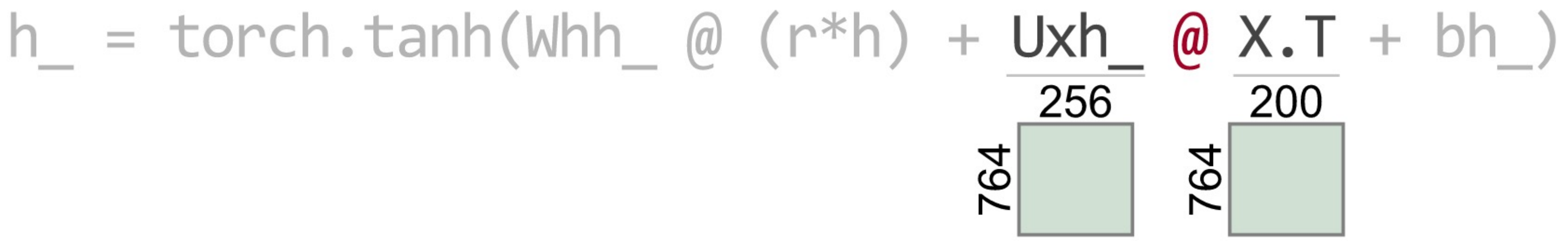
Better yet: make it obvious with a viz



```
Cause: @ on tensor operand Uxh_ w/shape [764, 256]
and operand X.T w/shape [764, 200]
```

(Notice the details like highlighting, red operator color, and de-highlighting)

See https://explained.ai/tensor-sensor/index.html

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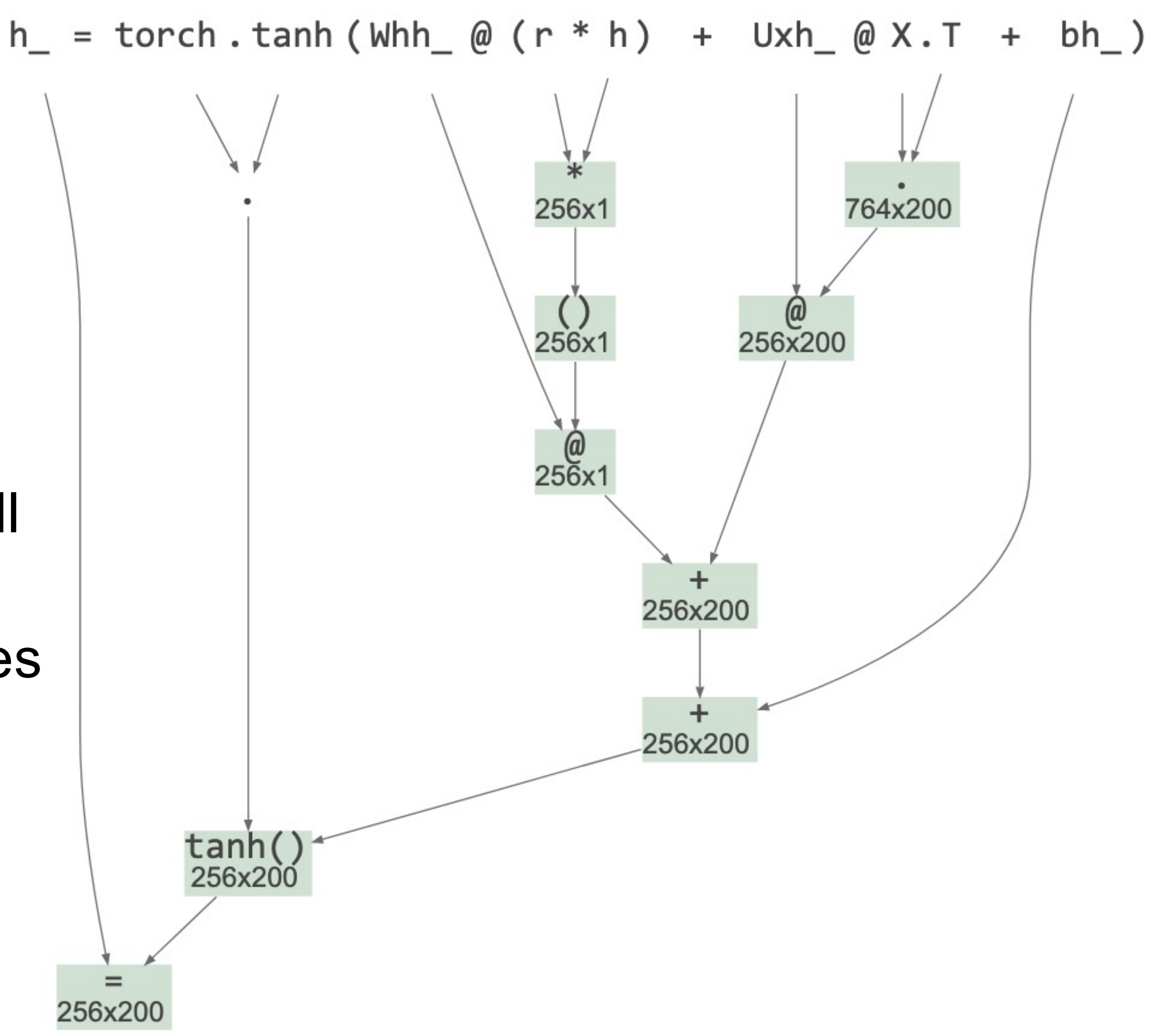
While we're at it… Aid for reading matrix code

- What do we care about when reading complex matrix expressions?
- We need the shape of all subexpressions
- Abstract syntax tree gives us an obvious viz with matrix dimensions



RNNs / neural nets are cloaked in mysticism

- I don't think the neural net analogy is helpful anymore
- The tangle of connections between neurons obscures rather than clarifies
- What exactly does that diagram portray?

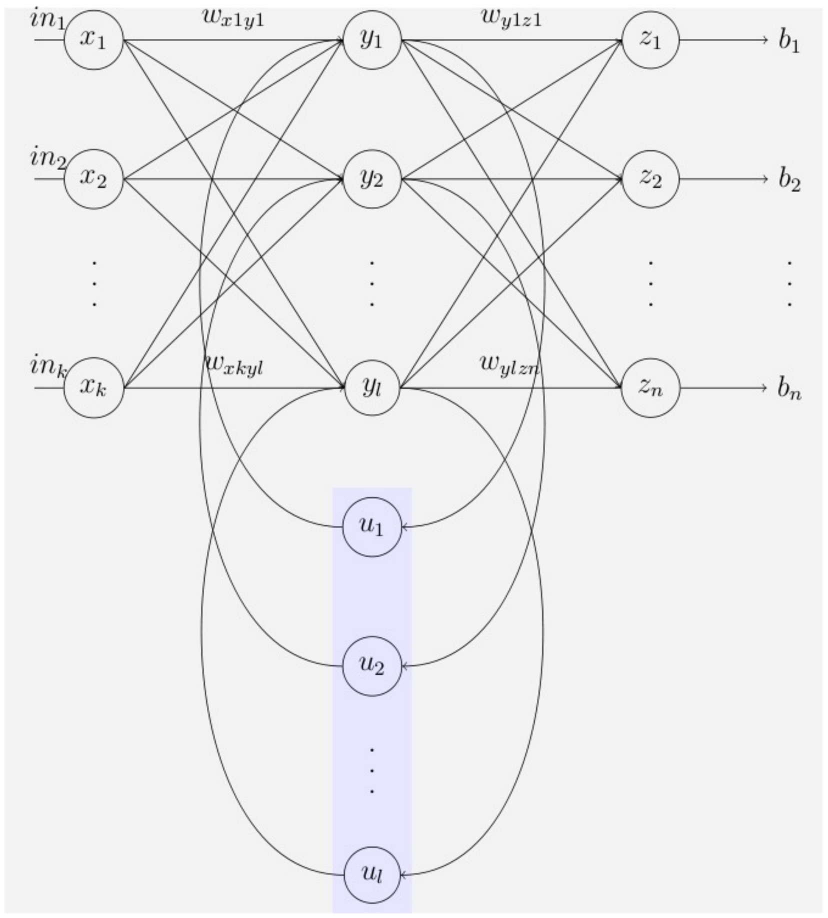


Image credit Fyedernoggersnodden https://en.wikipedia.org/wiki/Recurrent_neural_network

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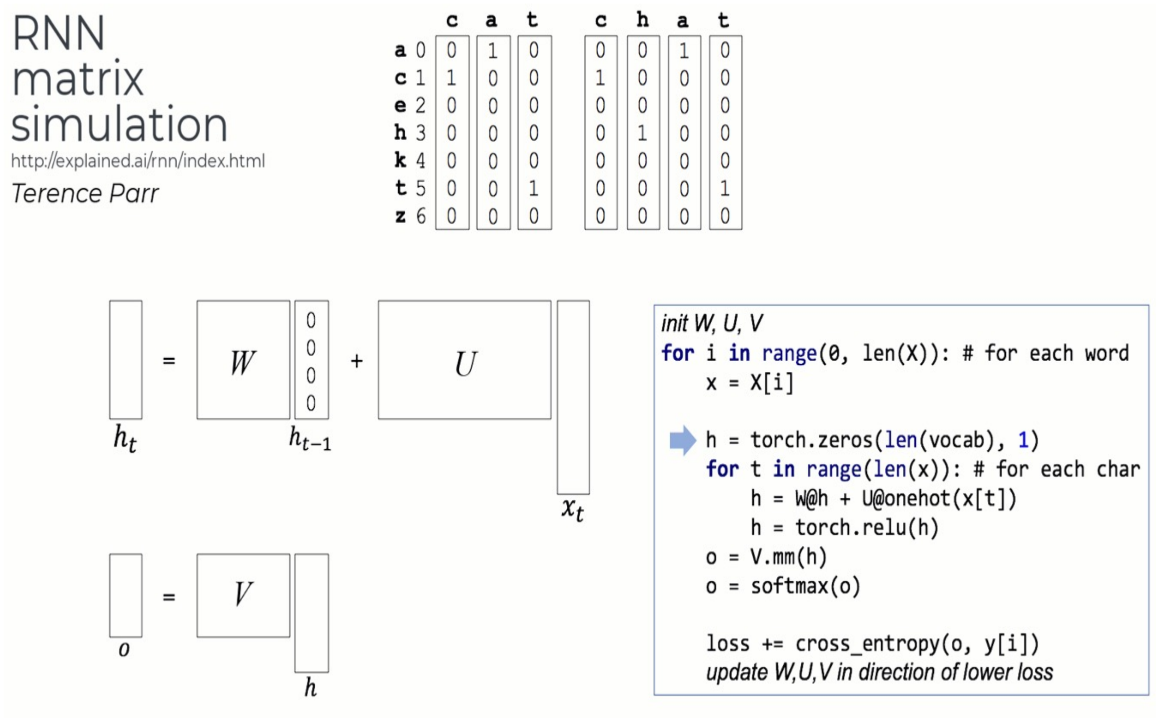
Strip away the mysticism

- What exactly is an RNN doing?
- It's just encoding symbols as vectors then aggregating them in a position-dependent way like a hash function for vectors; we use matrix transforms W, U and solve a classification problem to learn the parameters
- Animate the matrix algebra to make the implementation as concrete as possible
- (This animation was painful to build but is very helpful)

Classify cat words to language


RNN matrix simulation
http://explained.ai/rnn/index.html
Terence Parr
h_t = W h_{t-1} + U x_t
o = V h

		c	a	t	c	h	a	t
a	0	0	1	0	0	0	1	0
c	1	1	0	0	1	0	0	0
e	2	0	0	0	0	0	0	0
h	3	0	0	0	0	1	0	0
k	4	0	0	0	0	0	0	0
t	5	0	0	1	0	0	0	1
z	6	0	0	0	0	0	0	0

```
init W, U, V
for i in range(0, len(X)): # for each word
    x = X[i]

    h = torch.zeros(len(vocab), 1)
    for t in range(len(x)): # for each char
        h = W@h + U@onehot(x[t])
        h = torch.relu(h)
    o = V.mm(h)
    o = softmax(o)

    loss += cross_entropy(o, y[i])
    update W,U,V in direction of lower loss
```

(Notice weights W, U, V flash when updated)

See https://explained.ai/rnn/index.html

Be skeptical and confident: Sometimes everybody else is wrong and you are right

- Gini/var drop importance for random forests can be wildly wrong

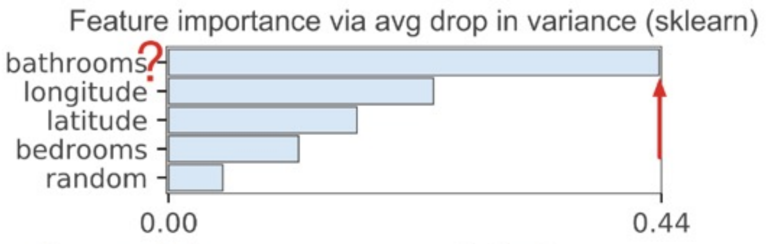


Figure 1(a). `scikit-learn` default importances for Random Forest **regressor** predicting apartment rental price from 4 features + a column of random numbers. Random column is last, as we would expect but the importance of the number of bathrooms for predicting price is highly suspicious.

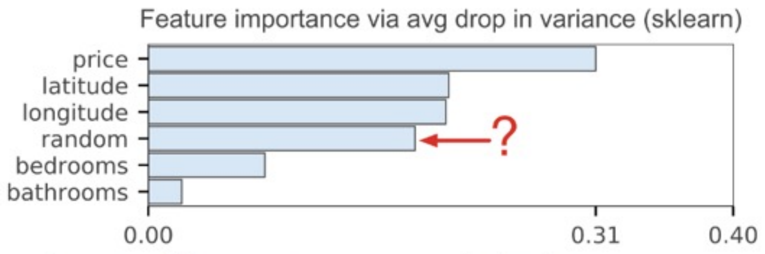


Figure 1(b). `scikit-learn` default importances for Random Forest **classifier** predicting apartment interest level (low, medium, high) using 5 features + a column of random numbers. Highly suspicious that random column is much more important than the number of bedrooms.

See https://explained.ai/rf-importance/index.html

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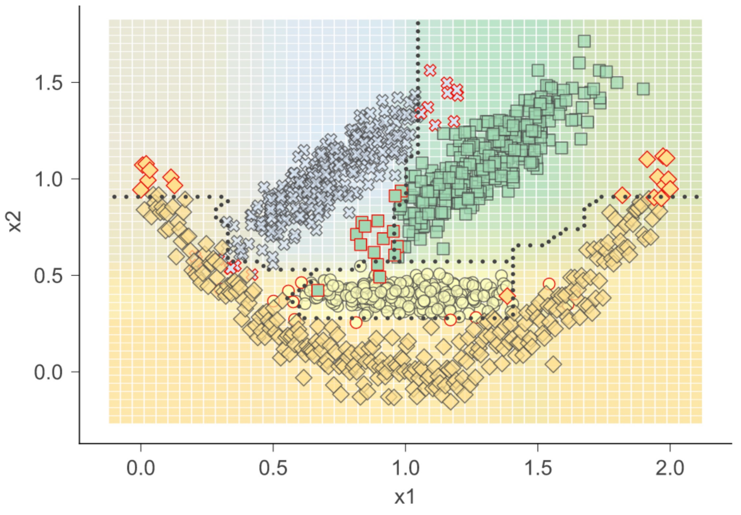
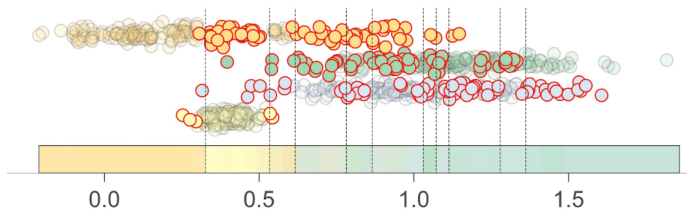
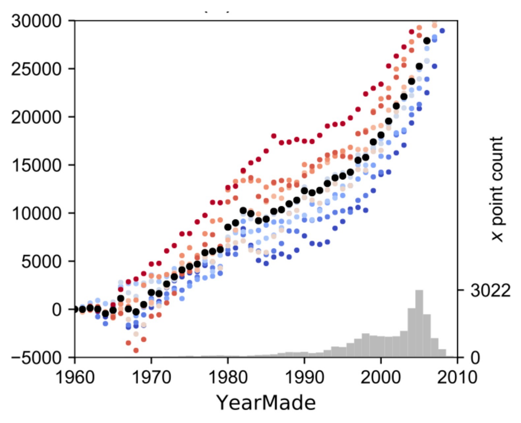
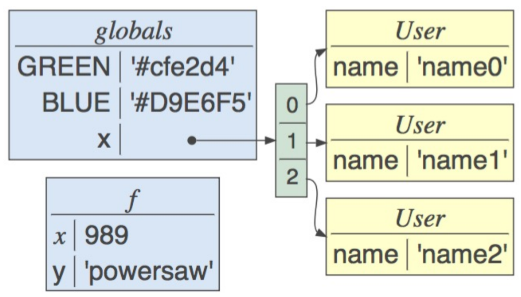
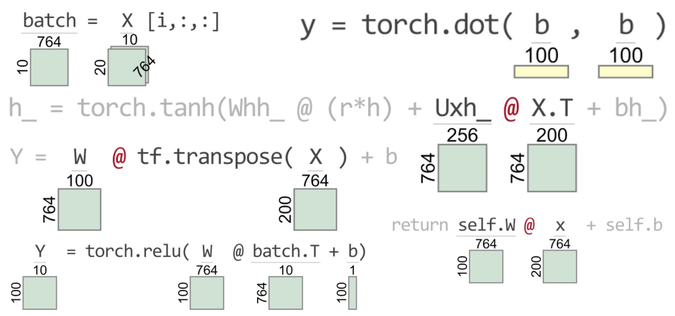
Engage the audience's visual cortex!











batch = X [i,:,:]
y = torch.dot(b , b)
h_ = torch.tanh(Whh_ @ (r*h) + Uxh_ @ X.T + bh_)
Y = W @ tf.transpose(X) + b
return self.W @ x + self.b
Y = torch.relu(W @ batch.T + b)

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Some final advice

6. When you feel coding or learning pain, work hard to erase it; crave beauty, excellence, and simplicity
7. Be tenacious; never let the computer win; bash your way to victory; deep understanding and clear visualizations often require pathological determination and a trail of dead code